23/43 SEARCH REQUEST FORM

Requesto	r's	BERCH	Serial Number:	01/106768
Date:	08	21/00 Phone:	47/8	Art Unit: 8 1624

Search Topic:

PTO-1590 (9-90)

Please write a detailed statement of search topic. Describe specifically as possible the subject matter to be searched. Define any terms that may have a special meaning. Give examples or relevent citations, authors, keywords, etc., if known. For sequences, please attach a copy of the sequence. You may include a copy of the broadest and/or most relevent claim(s).

Point of Contact: Mary Hale Technical Info. Specialist CM1 12D16 Tel: 308-4258

STAFF USE ONLY

-Date completed: 8 23	: Search Site	Vendors
Searcher: Many	STIC	IG.
Terminal time:	CM-1	(129,3) STN
Elapsed time: 5	Pre-S	Dialog
CPU time:	Type of Search	APS
Total time:	N.A. Sequence	Geninfo
Number of Searches:	. A.A. Sequence	SDC
Number of Databases:	Structure	DARC/Questel
	Bibliographic	Other

BEREH 381750

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 11, 2000

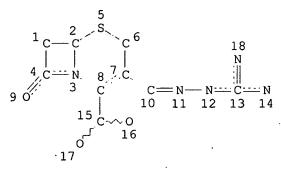
Please note that search-term pricing does apply when conducting ${\tt SmartSELECT}$ searches.

Structure search limits have been increased. See HELP SLIMIT for details.

=> d 13 que stat; d 1-148 ide cbib abs

L1

STR



NODE ATTRIBUTES:

NSPEC IS R AT 14 DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

L3 148 SEA FILE=REGISTRY SSS FUL L1

100.0% PROCESSED 422 ITERATIONS

DNS 148 ANSWERS

SEARCH TIME: 00.00.01

- L3 ANSWER 1 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 214055-89-7 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

7-[[(2Z)-(5-amino-1,2,4-thiadiazol-3-yl)[(fluoromethoxy)imino]acetyl]amino]-3-[(E)-[(imino-1-piperazinylmethyl)methylhydrazono]methyl]-8-oxo-, trihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)

FS STERÉOSEARCH

MF C19 H24 F N11 O5 S2 . 3 C1 H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry. Double bond geometry as shown.

3 HC1

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 A1 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GI

$$R^1$$
 V
 CO
 NH
 H_2N
 S
 N
 CO_2R^5
 R^3
 R^3
 R^4
 I

AB Synthesis of cephalosporins (I) [Rl = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

L3 ANSWER 2 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-86-4 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

7-[[(2Z)-(5-amino-1,2,4-thiadiazol-3-yl)[(fluoromethoxy)imino]acetyl]amino
]-3-[[(imino-1-piperazinylmethyl)hydrazono]methyl]-8-oxo-,
1-[[(1-methylethoxy)carbonyl]oxy]ethyl ester, dihydrochloride, (6R,7R)(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C24 H32 F N11 O8 S2 . 2 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

PAGE 2-A

● 2 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 A1 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GI

- AB Synthesis of cephalosporins (I) [Rl = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with
- 1-(1-methylhydrazino)iminomethylpiperaz ine dihydrochloride followed by chromatog.
- L3 ANSWER 3 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 214055-83-1 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
- 7-[[(2Z)-(5-amino-1,2,4-thiadiazol-3-yl)[(fluoromethoxy)imino]acetyl]amino]-3-[[(imino-1-piperazinylmethyl)hydrazono]methyl]-8-oxo-, (2,2-dimethyl-1-oxopropoxy)methyl ester, (6R,7R)- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH MF C24 H32 F N11 O7 S2
- SR CA
- LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates.

Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 A1 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GΙ

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = Prepared by M. Hale 308-4258

OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyliminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz

ine dihydrochloride followed by chromatog.

L3 ANSWER 4 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-82-0 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

3-[[[4-[amino(4-hydroxyphenyl)acetyl]-1-piperazinyl]iminomethyl]hydrazono]methyl]-7-[[(2Z)-(5-amino-1,2,4-thiadiazol-3-yl)[(fluoromethoxy)imino]acetyl]amino]-8-oxo-, (2,2-dimethyl-1-oxopropoxy)methyl ester, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C32 H39 F N12 O9 S2

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

PAGE 1-A

PAGE 1-B

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE) Prepared by M. Hale 308-4258

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates.

Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GI

$$R^{1}$$
 N
 $CO_{2}R^{5}$
 R^{3}
 R^{3}
 R^{3}
 R^{4}
 R^{4}

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyliminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

L3 ANSWER 5 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-81-9 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

MF C32 H39 F N12 O10 S2

SR CA

Prepared by M. Hale 308-4258

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

PAGE 1-B

- 1 REFERENCES IN FILE CA (1967 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GΙ

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

L3 ANSWER 6 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-80-8 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[[(2Z)-(2-amino-4-thiazolyl)[(fluoromethoxy)imino]acetyl]amino]-3[[(imino-1-piperazinylmethyl)hydrazono]methyl]-8-oxo-,
1-[[(1-methylethoxy)carbonyl]oxy]ethyl ester, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C25 H33 F N10 O8 S2

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry. Double bond geometry as described by E or Z.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 A1 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GΙ

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, Prepared by M. Hale 308-4258

aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

L3 ANSWER 7 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-79-5 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
3-[[(4-acetyl-1-piperazinyl)iminomethyl]hydrazono]methyl]-7-[[(2Z)-(5-amino-1,2,4-thiadiazol-3-yl)[(fluoromethoxy)imino]acetyl]amino]-8-oxo-,
1-[[(1-methylethoxy)carbonyl]oxy]ethyl ester, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C26 H34 F N11 O9 S2

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 A1 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, Prepared by M. Hale 308-4258

BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GΙ

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

L3 ANSWER 8 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-78-4 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

3-[[[4-[(2R)-2-amino-1-oxopropyl]-1-piperazinyl]iminomethyl]hydrazono]met hyl]-7-[[(2Z)-(2-amino-4-thiazolyl)(hydroxyimino)acetyl]amino]-8-oxo-, trihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C21 H27 N11 O6 S2 . 3 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

3 HC1

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GI

$$R^{1}$$
 V
 CO
 NH
 $H_{2}N$
 $CO_{2}R^{5}$
 R^{2}
 N
 R^{3}
 R^{4}
 I

Prepared by M. Hale 308-4258

- AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with
- 1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.
- L3 ANSWER 9 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 214055-77-3 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
- 3-[[[4-[(2S)-2-amino-1-oxopropyl]-1-piperazinyl]iminomethyl]hydrazono]met hyl]-7-[[(2Z)-(2-amino-4-thiazolyl)(hydroxyimino)acetyl]amino]-8-oxo-, trihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C21 H27 N11 O6 S2 . 3 Cl H
- SR CA
- LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

• 3 HCl

- 1 REFERENCES IN FILE CA (1967 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

Prepared by M. Hale 308-4258

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates.

Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GI

$$R^{1}$$
 V
 CO
 NH
 $H_{2}N$
 $CO_{2}R^{5}$
 R_{2}
 N
 R^{3}
 R^{4}
 I

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz ine dihydrochloride followed by chromatog.

L3 ANSWER 10 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-76-2 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

7-[[(2Z)-(5-amino-1,2,4-thiadiazol-3-yl)[(fluoromethoxy)imino]acetyl]amino

]-3-[[[imino[4-(3,4,5-trimethoxybenzoyl)-1-piperazinyl]methyl]hydrazono]methyl]-8-oxo-, dihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C28 H32 F N11 O9 S2 . 2 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry. Prepared by M. Hale 308-4258

Double bond geometry as described by E or Z.

● 2 HCl

PAGE 1-B

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). Prepared by M. Hale 308-4258

CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GI

$$R^{1}$$
 V
 CO
 NH
 $H_{2}N$
 $CO_{2}R^{5}$
 R^{2}
 N
 R^{3}
 R^{4}
 I

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

L3 ANSWER 11 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-75-1 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[[(2Z)-(2-amino-4-thiazolyl) (hydroxyimino)acetyl]amino]-3-[[[imino[4-(3,4,5-trimethoxybenzoyl)-1-piperazinyl]methyl]hydrazono]methyl]-8-oxo-,
dihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C28 H32 N10 O9 S2 . 2 Cl H

SR CA

LC. STN Files: CA, CAPLUS

Absolute stereochemistry. Double bond geometry as described by E or Z.

Prepared by M. Hale 308-4258

2 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GΙ

Prepared by M. Hale 308-4258

- AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with
- 1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.
- L3 ANSWER 12 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-74-0 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[(2Z)-(2-amino-4-thiazolyl) (hydroxyimino)acetyl]amino]-3-[[[[4-(cyclopropylcarbonyl)-1-piperazinyl]iminomethyl]hydrazono]methyl]-8-oxo-, dihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C22 H26 N10 O6 S2 . 2 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

OH O R R R NH NH NH
$$N$$

● 2 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted Prepared by M. Hale 308-4258

 ${\tt acylamino} \, ({\tt methylhydrazono}) \, {\tt methylcephalosporins} \, \, {\tt and} \, \, {\tt intermediates}. \, \\ {\tt Ascher}, \,$

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 A1 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GI

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyliminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

- L3 ANSWER 13 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 214055-73-9 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[(2Z)-(2-amino-4-thiazolyl) (hydroxyimino)acetyl]amino]-3-[[[[4-(3-carboxy-1-oxopropyl)-1-piperazinyl]iminomethyl]hydrazono]methyl]-8-oxo-, dihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C22 H26 N10 O8 S2 . 2 Cl H
- SR CA
- LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

● 2 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GΙ

$$R^{1}$$
 V
 CO
 NH
 $H_{2}N$
 $CO_{2}R^{5}$
 R^{2}
 N
 R^{3}
 R^{4}
 I

Prepared by M. Hale 308-4258

- AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyliminoacetic acid, reaction of this intermediate with
- 1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.
- L3 ANSWER 14 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 214055-72-8 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[(2Z)-(2-amino-4-thiazolyl)(hydroxyimino)acetyl]amino]-3-[[[[4-

FS STEREOSEARCH

MF C19 H25 N13 O5 S2 . 3 C1 H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

• 3 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

Prepared by M. Hale 308-4258

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino (methylhydrazono) methylcephalosporins and intermediates.

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 A1 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GI

$$R^{1}$$
 N
 $CO_{2}R^{5}$
 R^{3}
 R^{3}
 R^{4}
 R^{4}

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1, 2, 4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz ine dihydrochloride followed by chromatog.

L3 ANSWER 15 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-71-7 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

7-[[(2Z)-(5-amino-1,2,4-thiadiazol-3-yl)[(fluoromethoxy)imino]acetyl]amino]-3-[[[[4-[[[3-(dimethylamino)propyl]amino](ethylimino)methyl]-1piperazinyl]iminomethyl]hydrazono]methyl]-8-oxo-, trihydrochloride, (6R, 7R) - (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C26 H39 F N14 O5 S2 . 3 Cl H

SR CA

LC STN Files: CA, CAPLUS

Double bond geometry as described by E or Z.

PAGE 1-A

• 3 HCl

PAGE 1-B

(CH₂) 3 NMe₂

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael: Ludescher, Johannes; Hildebrandt, Prepared by M. Hale 308-4258 Page 79

Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GΙ

$$R^{1}$$
 V
 CO
 NH
 $H_{2}N$
 $CO_{2}R^{5}$
 R_{2}
 N
 R^{3}
 R^{4}
 T

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyliminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

L3 ANSWER 16 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-70-6 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

7-[[(2Z)-(5-amino-1,2,4-thiadiazol-3-yl)[(fluoromethoxy)imino]acetyl]amino

]-3-[[[imino[4-(iminohydrazinomethyl)-1-piperazinyl]methyl]hydrazono]methyl]-8-oxo-, trihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C19 H25 F N14 O5 S2 . 3 C1 H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

3 HCl

PAGE 1-B

^{_}NH2

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 A1 Prepared by M. Hale 308-4258 Page 81 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GΙ

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

L3 ANSWER 17 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-69-3 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[[[4-[(2R)-amino(4-hydroxyphenyl)acetyl]-1-piperazinyl]iminomethyl]hydrazono]methyl]-7-[[(2Z)-(5-amino-1,2,4-thiadiazol-3-yl)[(fluoromethoxy)imino]acetyl]amino]-8-oxo-, trihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C26 H29 F N12 O7 S2 . 3 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

FCH₂
$$\stackrel{\circ}{N}$$
 $\stackrel{\circ}{N}$ $\stackrel{\circ}{N}$

● 3 HC1

PAGE 1-B

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino (methylhydrazono) methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 A1 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GI

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

L3 ANSWER 18 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-68-2 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[[[4-[(2S,3S)-2-amino-3-methyl-1-oxopentyl]-1-piperazinyl]iminomethyl]hydrazono]methyl]-7-[[(2Z)-(5-amino-1,2,4-thiadiazol-3-yl)[(fluoromethoxy)imino]acetyl]amino]-8-oxo-, trihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C24 H33 F N12 O6 S2 . 3 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

• 3 HCl

PAGE 1-B

__Et

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher.

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, Prepared by M. Hale 308-4258

BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GΙ

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

L3 ANSWER 19 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-67-1 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

3-[[[[4-(aminoacetyl)-1-piperazinyl]iminomethyl]hydrazono]methyl]-7-[[(2Z)-

(5-amino-1,2,4-thiadiazol-3-yl)[(fluoromethoxy)imino]acetyl]amino]-8-oxo-, trihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C20 H25 F N12 O6 S2 . 3 C1 H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

● 3 HCl

PAGE 1-B

NH₂

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al Prepared by M. Hale 308-4258 Page 87 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GΙ

$$R1$$
 V
 CO
 NH
 H_2N
 CO_2R^5
 R_2
 N
 R_4
 R_4

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

L3 ANSWER 20 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-66-0 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

7-[[(2Z)-(5-amino-1,2,4-thiadiazol-3-yl)[(fluoromethoxy)imino]acetyl]amino
]-3-[[[imino[4-[(2S)-2-pyrrolidinylcarbonyl]-1piperazinyl]methyl]hydrazono]methyl]-8-oxo-, trihydrochloride, (6R,7R)(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C23 H29 F N12 O6 S2 . 3 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

• 3 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates.

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 A1 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GΙ

$$R^{1}$$
 V
 $CO_{2}R^{5}$
 R^{3}
 R^{3}
 R^{3}
 R^{3}
 R^{4}
 R^{4}

Prepared by M. Hale 308-4258

- AB Synthesis of cephalosporins (I) [Rl = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyliminoacetic acid, reaction of this intermediate with
- 1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.
- L3 ANSWER 21 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-65-9 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
3-[[(4-acetyl-1-piperazinyl)iminomethyl]hydrazono]methyl]-7-[[(2Z)-(5-amino-1,2,4-thiadiazol-3-yl)[(fluoromethoxy)imino]acetyl]amino]-8-oxo-,
dihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C20 H24 F N11 O6 S2 . 2 C1 H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry. Double bond geometry as described by E or Z.

● 2 HCl

1 REFERENCES IN FILE CAPILLS (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Prepared by M. Hale 308-4258

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 A1 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GI

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyliminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

L3 ANSWER 22 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-64-8 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

3-[[[[4-[2-(acetyloxy)benzoyl]-1-piperazinyl]iminomethyl]hydrazono]methyl]-

7-[[(2Z)-(5-amino-1,2,4-thiadiazol-3-yl)[(fluoromethoxy)imino]acetyl]amino]-8-oxo-, dihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C27 H28 F N11 O8 S2 . 2 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

● 2 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GI

Prepared by M. Hale 308-4258

- AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with
- 1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.
- L3 ANSWER 23 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 214055-63-7 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
- 7-[[(2Z)-(5-amino-1,2,4-thiadiazol-3-yl)[(fluoromethoxy)imino]acetyl]amino]-3-[[[imino[4-(phenoxyacetyl)-1-piperazinyl]methyl]hydrazono]methyl]-8-oxo-, dihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C26 H28 F N11 O7 S2 . 2 C1 H
- SR CA
- LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

PAGE 1-A

● 2 HCl

[→] OPh

- 1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)
- REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates.

Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt,
Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 A1
19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG,
BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU,
ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG,
MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM,
TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM;
RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB,
GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English).
CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT
1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GI

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, Prepared by M. Hale 308-4258

alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

L3 ANSWER 24 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-62-6 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[(2Z)-(2-amino-4-thiazolyl)(hydroxyimino)acetyl]amino]-3-[[[(4-(2,3-

FS STEREOSEARCH

MF C21 H26 N10 O8 S2 . 2 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

● 2 · HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael: Ludescher, Johannes; Hildebrandt, Prepared by M. Hale 308-4258

Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 A1 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GΙ

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

L3 ANSWER 25 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-61-5 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

7-[[(2Z)-(2-amino-4-thiazolyl)(hydroxyimino)acetyl]amino]-3-[[[imino[4-(1-oxooctyl)-1-piperazinyl]methyl]hydrazono]methyl]-8-oxo-, dihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C26 H36 N10 O6 S2 . 2 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

● 2 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GI

Prepared by M. Hale 308-4258

- AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with
- 1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.
- L3 ANSWER 26 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 214055-60-4 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
- 7-[[(2Z)-(2-amino-4-thiazolyl)(hydroxyimino)acetyl]amino]-3-[[[imino[4-(1-oxohexadecyl)-1-piperazinyl]methyl]hydrazono]methyl]-8-oxo-, dihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C34 H52 N10 O6 S2 . 2 Cl H
- SR CA
- LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

● 2 HCl

- 1 REFERENCES IN FILE CA (1967 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

Prepared by M. Hale 308-4258

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates.

Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GI

$$R^{1}$$
 N
 $CO_{2}R^{5}$
 R^{3}
 R^{3}
 R^{3}
 R^{4}
 R^{4}

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyliminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

L3 ANSWER 27 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-59-1 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

7-[[(2Z)-(2-amino-4-thiazolyl)(hydroxyimino)acetyl]amino]-3-[[[imino[4-(1-oxooctadecyl)-1-piperazinyl]methyl]hydrazono]methyl]-8-oxo-, dihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C36 H56 N10 O6 S2 . 2 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z. Prepared by M. Hale 308-4258

2 HC1

- 1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE) .
- REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 A1 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GΙ

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

L3 ANSWER 28 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-58-0 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

7-[[(2Z)-(2-amino-4-thiazolyl)(hydroxyimino)acetyl]amino]-3-[[[imino[4-(1-oxoheptyl)-1-piperazinyl]methyl]hydrazono]methyl]-8-oxo-, dihydrochloride,

(6R, 7R) - (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C25 H34 N10 O6 S2 . 2 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

● 2 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GI

$$R^{1}$$
 V
 CO
 NH
 $H_{2}N$
 $CO_{2}R^{5}$
 R^{2}
 N
 R^{3}
 R^{4}
 I

Prepared by M. Hale 308-4258

- AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with
- 1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.
- L3 ANSWER 29 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 214055-57-9 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 3-[[[4-[(2S,3S)-2-amino-3-methyl-1-oxopentyl]-1piperazinyl]iminomethyl]hydrazono]methyl]-7-[[(2Z)-(2-amino-4thiazolyl)(hydroxyimino)acetyl]amino]-8-oxo-, trihydrochloride, (6R,7R)(9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C24 H33 N11 O6 S2 . 3 C1 H
- SR CA
- LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

● 3 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

Prepared by M. Hale 308-4258

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates.

Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GΙ

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz

ine dihydrochloride followed by chromatog.

L3 ANSWER 30 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-56-8 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
3-[[[4-[(2S)-2-amino-4-carboxy-1-oxobutyl]-1piperazinyl]iminomethyl]hydrazono]methyl]-7-[[(2Z)-(2-amino-4-thiazolyl)(hydroxyimino)acetyl]amino]-8-oxo-, dihydrochloride, (6R,7R)-(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C23 H29 N11 O8 S2 . 2 C1 H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z. Prepared by M. Hale 308-4258

2 HC1

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GΙ

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1, 2, 4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz ine dihydrochloride followed by chromatog.

ANSWER 31 OF 148 REGISTRY COPYRIGHT 2000 ACS L3

214055-55-7 REGISTRY RN

5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, CN 3-[[[4-(2S)-2-amino-5-(aminoiminomethyl)amino]-1-oxopentyl]-1piperazinyl]iminomethyl]hydrazono]methyl]-7-[[(2Z)-(2-amino-4thiazolyl) (hydroxyimino)acetyl]amino]-8-oxo-, tetrahydrochloride,

(6R, 7R) -

(CA INDEX NAME) (9CI)

STEREOSEARCH FS

MF C24 ·H34 N14 O6 S2 . 4 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry. Double bond geometry as described by E or Z.

• 4 HCl

PAGE 1-B

_NH2

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, Prepared by M. Hale 308-4258

MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GI

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz ine dihydrochloride followed by chromatog.

L3 ANSWER 32 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-54-6 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[(2Z)-(2-amino-4-thiazolyl)(hydroxyimino)acetyl]amino]-3-[[[[4-(hydroxyacetyl)-1-piperazinyl]iminomethyl]hydrazono]methyl]-8-oxo-, dihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C20 H24 N10 O7 S2 . 2 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry. Double bond geometry as described by ${\tt E}$ or ${\tt Z}$.

• 2 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GI

$$R^{1}$$
 V
 CO
 NH
 $H_{2}N$
 $CO_{2}R^{5}$
 R^{2}
 N
 R^{3}
 R^{4}
 R^{4}

Prepared by M. Hale 308-4258

- AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with
- 1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.
- L3 ANSWER 33 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 214055-53-5 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 3-[[[4-[(2S)-2-amino-5-[[imino(nitroamino)methyl]amino]-1-oxopentyl]-1piperazinyl]iminomethyl]hydrazono]methyl]-7-[[(2Z)-(2-amino-4thiazolyl)(hydroxyimino)acetyl]amino]-8-oxo-, trihydrochloride, (6R,7R)(9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C24 H33 N15 O8 S2 . 3 Cl H
- SR CA
- LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

PAGE 1-A

• 3 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 A1 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GI

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, Prepared by M. Hale 308-4258

NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz

ine dihydrochloride followed by chromatog.

L3 ANSWER 34 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-52-4 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[[[4-[(2R)-amino(4-hydroxyphenyl)acetyl]-1-

piperazinyl]iminomethyl]hydrazono]methyl]-7-[[(2Z)-(2-amino-4-

thiazolyl) (hydroxyimino)acetyl]amino]-8-oxo-, trihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C26 H29 N11 O7 S2 . 3 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

• 3 HCl

PAGE 1-B

__ OH

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates.

Ascher

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 A1 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GI

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

L3 ANSWER 35 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-51-3 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

3-[[[4-[(2R)-aminophenylacetyl]-1-piperazinyl]iminomethyl]hydrazono]methy 1]-7-[[(2Z)-(2-amino-4-thiazolyl)(hydroxyimino)acetyl]amino]-8-oxo-, trihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

Prepared by M. Hale 308-4258

MF C26 H29 N11 O6 S2 . 3 C1 H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry. Double bond geometry as described by E or Z.

● 3 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino (methylhydrazono) methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GΙ

$$R^{1}$$
 V
 CO
 NH
 $H_{2}N$
 $CO_{2}R^{5}$
 R_{2}
 N
 R^{3}
 R^{4}
 I

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

L3 ANSWER 36 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-50-2 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

3-[[[4-[2-(acetyloxy)benzoyl]-1-piperazinyl]iminomethyl]hydrazono]methyl]7-[[(2Z)-(2-amino-4-thiazolyl)(hydroxyimino)acetyl]amino]-8-oxo-,
dihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C27 H28 N10 O8 S2 . 2 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

● 2 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GI

$$R^{1}$$
 V
 CO
 NH
 $H_{2}N$
 $CO_{2}R^{5}$
 R^{2}
 N
 R^{3}
 R^{4}
 I

Prepared by M. Hale 308-4258

- AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with
- 1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.
- L3 ANSWER 37 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 214055-49-9 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[(2Z)-(2-amino-4-thiazolyl)(hydroxyimino)acetyl]amino]-3-[[[imino[4-
- [(2S)-2-pyrrolidinylcarbonyl]-1-piperazinyl]methyl]hydrazono]methyl]-8-oxo-, trihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C23 H29 N11 O6 S2 . 3 Cl H
- SR CA
- LC STN Files: CA, CAPLUS

Absolute stereochemistry. Double bond geometry as described by E or Z.

$$\begin{array}{c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & &$$

• 3 HCl

- 1 REFERENCES IN FILE CA (1967 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

Prepared by M. Hale 308-4258

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates.

Ascher

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GI

$$R^{1}$$
 V
 CO
 NH
 $H_{2}N$
 $CO_{2}R^{5}$
 R^{2}
 N
 R^{3}
 R^{4}
 I

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

L3 ANSWER 38 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-48-8 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[[(2Z)-(2-amino-4-thiazolyl)(hydroxyimino)acetyl]amino]-3-[[[imino[4-(phenoxyacetyl)-1-piperazinyl]methyl]hydrazono]methyl]-8-oxo-,
dihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C26 H28 N10 O7 S2 . 2 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

2 HC1

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GΙ

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- AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with
- 1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.
- L3 ANSWER 39 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 214055-47-7 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 7-[[(2Z)-(2-amino-4-thiazolyl)(hydroxyimino)acetyl]amino]-3-[[[[4[(dimethylamino)carbonyl]-1-piperazinyl]iminomethyl]hydrazono]methyl]-8oxo-, dihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C21 H27 N11 O6 S2 . 2 Cl H
- SR CA
- LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

● 2 HCl

- 1 REFERENCES IN FILE CA (1967 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

Prepared by M. Hale 308-4258

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates.

Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GΙ

$$R^{1}$$
 V
 CO
 NH
 $H_{2}N$
 $CO_{2}R^{5}$
 R_{2}
 N
 R^{3}
 R^{4}
 I

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz ine dihydrochloride followed by chromatog.

L3 ANSWER 40 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-46-6 REGISTRY

amino-4-thiazolyl) (hydroxyimino) acetyl]-1-piperazinyl]iminomethyl]hydrazon
o]methyl]-8-oxo-, trihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C23 H25 N13 O7 S3 . 3 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z. Prepared by M. Hale 308-4258

● 3 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 A1 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GΙ

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

L3 ANSWER 41 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-45-5 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[(2Z)-(2-amino-4-thiazolyl)(hydroxyimino)acetyl]amino]-3-[[[imino[4-(phenylacetyl)-1-piperazinyl]methyl]hydrazono]methyl]-8-oxo-, dihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C26 H28 N10 O6 S2 . 2 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

● 2 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GĮ

$$R^{1}$$
 V
 CO
 NH
 $H_{2}N$
 $CO_{2}R^{5}$
 R^{2}
 N
 R^{3}
 R^{4}
 I

Prepared by M. Hale 308-4258

- AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with
- 1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.
- L3 ANSWER 42 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 214055-44-4 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 3-[[(4-acetyl-1-piperazinyl)iminomethyl]hydrazono]methyl]-7-[[(2Z)-(2-amino-4-thiazolyl)(hydroxyimino)acetyl]amino]-8-oxo-, dihydrochloride,
 (6R,7R)- (9CI) (CA INDEX NAME)
- FS . STEREOSEARCH
- MF C20 H24 N10 O6 S2 . 2 Cl H
- SR CA
- LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

• 2 HCl

- 1 REFERENCES IN FILE CA (1967 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Prepared by M. Hale 308-4258

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GI

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

L3 ANSWER 43 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-43-3 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

7-[[(2Z)-(2-amino-4-thiazolyl)(hydroxyimino)acetyl]amino]-3-[[(4-benzoyl-1-piperazinyl)iminomethyl]hydrazono]methyl]-8-oxo-, dihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C25 H26 N10 O6 S2 . 2 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry. Double bond geometry as described by E or Z.

2 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GΙ

$$R^{1}$$
 V
 CO
 NH
 H
 S
 $CO_{2}R^{5}$
 R^{2}
 N
 R^{3}
 R^{4}
 I

Prepared by M. Hale 308-4258

- AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with
- 1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.
- L3 ANSWER 44 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 214055-42-2 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

(6R, 7R) - (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C20 H25 N11 O6 S2 . 3 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

• 3 HCl

1 REFERENCES IN FILE CA (1967 TO DATE) .

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

Prepared by M. Hale 308-4258

Page 128

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates.

Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GI

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

L3 ANSWER 45 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-41-1 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[[(2Z)-(2-amino-4-thiazolyl)(hydroxyimino)acetyl]amino]-3-[[[[4-(ethoxycarbonyl)-1-piperazinyl]iminomethyl]hydrazono]methyl]-8-oxo-,
dihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C21 H26 N10 O7 S2 . 2 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

● 2 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GI

Page 130

- AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with
- .1-(1-methylhydrazino)iminomethylpiperaz ine dihydrochloride followed by chromatog.
- L3 ANSWER 46 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 214055-40-0 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
- 7-[[(2Z)-(5-amino-1,2,4-thiadiazol-3-yl)[(fluoromethoxy)imino]acetyl]amino
-]-3-[[(imino-1-piperazinylmethyl)[(3,4,5-trimethoxyphenyl)methyl]hydrazono]methyl]-8-oxo-, trihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C28 H34 F N11 O8 S2 . 3 C1 H
- SR CA
- LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

PAGE 1-A

3 HC1

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates.

Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 A1 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GΙ

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyliminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

- L3 ANSWER 47 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 214055-39-7 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, Prepared by M. Hale 308-4258

'7~[[(2Z)-(5-amino-1,2,4-thiadiazol-3-yl)[(fluoromethoxy)imino]acetyl]amino

]-3-[[(imino-1-piperazinylmethyl)[(4-methoxyphenyl)methyl]hydrazono]methyl]-8-oxo-, trihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C26 H30 F N11 O6 S2 . 3 C1 H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry. Double bond geometry as described by E or Z.

• 3 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GI

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

L3 ANSWER 48 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-38-6 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

7-[[(2Z)-(5-amino-1,2,4-thiadiazol-3-yl)[(fluoromethoxy)imino]acetyl]amino]-3-[[methyl[(methylimino)-1-piperazinylmethyl]hydrazono]methyl]-8-oxo-, monohydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C20 H26 F N11 O5 S2 . C1 H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

) HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GΙ

$$R^{1}$$
 V
 CO
 NH
 $H_{2}N$
 $CO_{2}R^{5}$
 R^{2}
 N
 R^{3}
 R^{4}
 I

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = Prepared by M. Hale 308-4258 Page 135

H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyliminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

L3 ANSWER 49 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-37-5 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

7-[[(2Z)-(5-amino-1,2,4-thiadiazol-3-yl)[(fluoromethoxy)imino]acetyl]amino]-3-[[(imino-1-piperazinylmethyl)-2-propenylhydrazono]methyl]-8-oxo-, trihydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C21 H26 F N11 O5 S2 . 3 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

● 3 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael: Ludescher, Johannes; Hildebrandt, Prepared by M. Hale 308-4258

Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 A1 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GI

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

L3 ANSWER 50 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-36-4 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

7-[[(2Z)-(5-amino-1,2,4-thiadiazol-3-yl)[(fluoromethoxy)imino]acetyl]amino]-3-[[[(ethylimino)-1-piperazinylmethyl]methylhydrazono]methyl]-8-oxo-, monohydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C21 H28 F N11 O5 S2 . Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

● HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 Al 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GΙ

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = Prepared by M. Hale 308-4258 Page 138

H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

L3 ANSWER 51 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-35-3 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

7-[[(2Z)-(5-amino-1,2,4-thiadiazol-3-yl)[(fluoromethoxy)imino]acetyl]amino]-3-[[ethyl(imino-1-piperazinylmethyl)hydrazono]methyl]-8-oxo-, monohydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C20 H26 F N11 O5 S2 . C1 H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry. Double bond geometry as described by E or Z.

• HCl

1 REFERENCES IN FILE CA (1967 TO DATE) 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Prepared by M. Hale 308-4258 Page 139

Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 A1 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GΙ

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

L3 ANSWER 52 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 214055-34-2 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

7-[[(2Z)-(5-amino-1,2,4-thiadiazol-3-yl)[(fluoromethoxy)imino]acetyl]amino]-3-[(E)-[(imino-1-piperazinylmethyl)methylhydrazono]methyl]-8-oxo-, monohydrochloride, (6R,7R)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C19 H24 F N11 O5 S2 . C1 H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry. Double bond geometry as shown.

• HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted acylamino(methylhydrazono)methylcephalosporins and intermediates. Ascher,

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 A1 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GΙ

$$R^{1}$$
 V
 CO
 NH
 $H_{2}N$
 $CO_{2}R^{5}$
 R^{2}
 N
 R^{3}
 R^{4}
 I

AB Synthesis of cephalosporins (I) [R1 = H, acyl carboxyl, alkyl; R2, R3 = Prepared by M. Hale 308-4258 Page 141

H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

L3 ANSWER 53 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 184943-50-8 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[[(5-amino-1,2,4-thiadiazol-3-yl)[(fluoromethoxy)imino]acetyl]amino]-3[[(imino-1-piperazinylmethyl)hydrazono]methyl]-8-oxo-,
[6R-[6.alpha.,7.beta.(Z)]]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C18 H22 F N11 O5 S2

CI COM

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:47035 Antibacterial cephalosporins. Ascher, Gerd; Ludescher, Johannes (Biochemie Gesellschaft Mbh, Austria; Ascher, Gerd; Ludescher, Johannes). PCT Int. Appl. WO 9635692 A1 19961114, 124 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN,

CZ,

DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1996-EP2023 19960510. PRIORITY: AT 1995-794 19950511; AT 1995-992 Prepared by M. Hale 308-4258

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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
AΒ
     Compds. of formula I (R1 = H or ester moiety, R2 = OY, NR4R5, N:R6, Y =
Η,
     alkyl, alkenyl, acyl, carbamoyl, aryl, R4 = H, alkyl, alkenyl,
cycloalkyl,
     aryl, acyl, heterocyclyl, R5 = H, alkyl, alkenyl, cycloalkyl, aryl,
     heterocyclyl, C(SR7):NR8, C(NR9R10):Z, CR11:Z, R7 = alkyl or aryl, R8 =
Η,
     cycloalkyl, alkyl, R9 = H or alkyl, R10 = H, alkyl, OH, NH2, Ph, alkenyl,
     cycloalkyl, aryl, heterocyclyl, N:CHPhe, Phe = aryl, R9 and R10 together
     with nitrogen form a heterocyclyl, Z = O, S, NR13, R13 = H, alkyl or
     cycloalkyl, R11 = H, alkyl, aryl, cycloalkyl, or heterocyclyl, R4 and R5
     together with nitrogen form a heterocyclyl, R6 = heterocyclyl, Ac = Ac1,
     COCZ1:CZ2Z3, COCZ1:BDZ4, B = N, CH, Z1 = aryl, cycloalkyl, 1,4-hexadienyl
     or heterocyclyl, Z2 = H, alkyl, CH2CO2Z5, Z5 = H, alkyl, cycloalkyl, Z3 =
     H, alkyl, Z4 = H or org. radical, D = O or CH2), were prepd. thereof for
     use as pharmaceuticals, i.e. as antibacterial agents. Thus, II was
    via condensation of formylcephemcarboxylic acid deriv. III in 4% aq. MeCN
     with quanidine IV in 1-2 N HCl. II has an MHK of 0.01 .mu.q/mL vs.
     Streptococcus pneumoniae (strain ATCC 49619) compared to 0.02 .mu.g/mL
for
     ceftriaxone.
L3
    ANSWER 54 OF 148 REGISTRY COPYRIGHT 2000 ACS
     184943-49-5 REGISTRY
RN
CN
     5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
     7-[[(2-amino-4-thiazolyl)(hydroxyimino)acetyl]amino]-3-[[(imino-1-
    piperazinylmethyl)hydrazono]methyl]-8-oxo-, [6R-[6.alpha.,7.beta.(Z)]]-
     (9CI)
           (CA INDEX NAME)
FS
     STEREOSEARCH
MF
     C18 H22 N10 O5 S2
CI
    COM
SR
     CA
LC
     STN Files:
                  CA, CAPLUS
Absolute stereochemistry.
```

Double bond geometry as described by E or Z.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:47035 Antibacterial cephalosporins. Ascher, Gerd; Ludescher, Johannes (Biochemie Gesellschaft Mbh, Austria; Ascher, Gerd; Ludescher, Johannes). PCT Int. Appl. WO 9635692 Al 19961114, 124 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN,

CZ,

DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1996-EP2023 19960510. PRIORITY: AT 1995-794 19950511; AT 1995-992 19950612; AT 1996-698 19960417; AT 1996-733 19960423.

GΙ

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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. of formula I (R1 = H or ester moiety, R2 = OY, NR4R5, N:R6, Y = H,

alkyl, alkenyl, acyl, carbamoyl, aryl, R4 = H, alkyl, alkenyl,
cycloalkyl,

aryl, acyl, heterocyclyl, R5 = H, alkyl, alkenyl, cycloalkyl, aryl,
heterocyclyl, C(SR7):NR8, C(NR9R10):Z, CR11:Z, R7 = alkyl or aryl, R8 =

cycloalkyl, alkyl, R9 = H or alkyl, R10 = H, alkyl, OH, NH2, Ph, alkenyl, cycloalkyl, aryl, heterocyclyl, N:CHPhe, Phe = aryl, R9 and R10 together with nitrogen form a heterocyclyl, Z = O, S, NR13, R13 = H, alkyl or cycloalkyl, R11 = H, alkyl, aryl, cycloalkyl, or heterocyclyl, R4 and R5 together with nitrogen form a heterocyclyl, R6 = heterocyclyl, Ac = Ac1, COCZ1:CZ2Z3, COCZ1:BDZ4, B = N, CH, Z1 = aryl, cycloalkyl, 1,4-hexadienyl or heterocyclyl, Z2 = H, alkyl, CH2CO2Z5, Z5 = H, alkyl, cycloalkyl, Z3 = H, alkyl, Z4 = H or org. radical, D = O or CH2), were prepd. thereof for use as pharmaceuticals, i.e. as antibacterial agents. Thus, II was prepd.

via condensation of formylcephemcarboxylic acid deriv. III in 4% aq. MeCN Prepared by M. Hale 308-4258 Page 144 with guanidine IV in 1-2 N HCl. II has an MHK of 0.01 .mu.g/mL vs. Streptococcus pneumoniae (strain ATCC 49619) compared to 0.02 .mu.g/mL $^{\prime\prime}$

for ceftriaxone.

L3 ANSWER 55 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 184942-76-5 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[[(5-amino-1,2,4-thiadiazol-3-yl)[(fluoromethoxy)imino]acetyl]amino]-3[[(imino-1-piperazinylmethyl)hydrazono]methyl]-8-oxo-, trihydrochloride,
[6R-[6.alpha.,7.beta.(Z)]]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C18 H22 F N11 O5 S2 . 3 Cl H

SR CA

LC STN Files: CA, CAPLUS

CRN (184943-50-8)

Absolute stereochemistry. Double bond geometry as described by E or Z.

• 3 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:47035 Antibacterial cephalosporins. Ascher, Gerd; Ludescher, Johannes (Biochemie Gesellschaft Mbh, Austria; Ascher, Gerd; Ludescher, Johannes). PCT Int. Appl. WO 9635692 Al 19961114, 124 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ,

DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1996-EP2023 19960510. PRIORITY: AT 1995-794 19950511; AT 1995-992 Prepared by M. Hale 308-4258

```
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT * AB Compds. of formula I (R1 = H or ester moiety, R2 = OY, NR4R5, N:R6, Y = H,
```

alkyl, alkenyl, acyl, carbamoyl, aryl, R4 = H, alkyl, alkenyl, cycloalkyl,

aryl, acyl, heterocyclyl, R5 = H, alkyl, alkenyl, cycloalkyl, aryl, heterocyclyl, C(SR7):NR8, C(NR9R10):Z, CR11:Z, R7 = alkyl or aryl, R8 =

H,

cycloalkyl, alkyl, R9 = H or alkyl, R10 = H, alkyl, OH, NH2, Ph, alkenyl, cycloalkyl, aryl, heterocyclyl, N:CHPhe, Phe = aryl, R9 and R10 together with nitrogen form a heterocyclyl, Z = O, S, NR13, R13 = H, alkyl or cycloalkyl, R11 = H, alkyl, aryl, cycloalkyl, or heterocyclyl, R4 and R5 together with nitrogen form a heterocyclyl, R6 = heterocyclyl, Ac = Ac1, COCZ1:CZ2Z3, COCZ1:BDZ4, B = N, CH, Z1 = aryl, cycloalkyl, 1,4-hexadienyl or heterocyclyl, Z2 = H, alkyl, CH2CO2Z5, Z5 = H, alkyl, cycloalkyl, Z3 = H, alkyl, Z4 = H or org. radical, D = O or CH2), were prepd. thereof for use as pharmaceuticals, i.e. as antibacterial agents. Thus, II was

via condensation of formylcephemcarboxylic acid deriv. III in 4% aq. MeCN with guanidine IV in 1-2 N HCl. II has an MHK of 0.01 .mu.g/mL vs. Streptococcus pneumoniae (strain ATCC 49619) compared to 0.02 .mu.g/mL

for

ceftriaxone.

- L3 ANSWER 56 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 184942-65-2 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[(2-amino-4-thiazolyl)(hydroxyimino)acetyl]amino]-3-[[(imino-1-piperazinylmethyl)methylhydrazono]methyl]-8-oxo-, trihydrochloride, [6R-[6.alpha.,7.beta.(Z)]]- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C19 H24 N10 O5 S2 . 3 Cl H
- SR CA
- LC STN Files: CA, CAPLUS

Absolute stereochemistry. Double bond geometry as described by E or Z.

3 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:47035 Antibacterial cephalosporins. Ascher, Gerd;
Ludescher, Johannes (Biochemie Gesellschaft Mbh, Austria; Ascher, Gerd;
Ludescher, Johannes). PCT Int. Appl. WO 9635692 Al 19961114, 124 pp.
DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN,
CZ,
DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS.

DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1996-EP2023 19960510. PRIORITY: AT 1995-794 19950511; AT 1995-992 19950612; AT 1996-698 19960417; AT 1996-733 19960423.

GΙ

Η,

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. of formula I (R1 = H or ester moiety, R2 = OY, NR4R5, N:R6, Y = H,

alkyl, alkenyl, acyl, carbamoyl, aryl, R4 = H, alkyl, alkenyl,
cycloalkyl,

aryl, acyl, heterocyclyl, R5 = H, alkyl, alkenyl, cycloalkyl, aryl, heterocyclyl, C(SR7):NR8, C(NR9R10):Z, CR11:Z, R7 = alkyl or aryl, R8 =

cycloalkyl, alkyl, R9 = H or alkyl, R10 = H, alkyl, OH, NH2, Ph, alkenyl, cycloalkyl, aryl, heterocyclyl, N:CHPhe, Phe = aryl, R9 and R10 together with nitrogen form a heterocyclyl, Z = O, S, NR13, R13 = H, alkyl or cycloalkyl, R11 = H, alkyl, aryl, cycloalkyl, or heterocyclyl, R4 and R5 together with nitrogen form a heterocyclyl, R6 = heterocyclyl, Ac = Ac1, COCZ1:CZ2Z3, COCZ1:BDZ4, B = N, CH, Z1 = aryl, cycloalkyl, 1,4-hexadienyl Prepared by M. Hale 308-4258

or heterocyclyl, Z2 = H, alkyl, CH2CO2Z5, Z5 = H, alkyl, cycloalkyl, Z3 = H, alkyl, Z4 = H or org. radical, D = O or CH2), were prepd. thereof for use as pharmaceuticals, i.e. as antibacterial agents. Thus, II was prepd.

via condensation of formylcephemcarboxylic acid deriv. III in 4% aq. MeCN with guanidine IV in 1-2 N HCl. II has an MHK of 0.01 .mu.g/mL vs. Streptococcus pneumoniae (strain ATCC 49619) compared to 0.02 .mu.g/mL

for ceftriaxone.

L3 ANSWER 57 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 184942-59-4 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

7-[[(2-amino-4-thiazolyl)(hydroxyimino)acetyl]amino]-3-[[[imino(4-methyl-1-piperazinyl)methyl]hydrazono]methyl]-8-oxo-, trihydrochloride, [6R-[6.alpha.,7.beta.(2)]]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C19 H24 N10 O5 S2 . 3 Cl H

SR CA.

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

• 3 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:47035 Antibacterial cephalosporins. Ascher, Gerd;
Ludescher, Johannes (Biochemie Gesellschaft Mbh, Austria; Ascher, Gerd;
Ludescher, Johannes). PCT Int. Appl. WO 9635692 A1 19961114, 124 pp.
DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN,
CZ,
Prepared by M. Hale 308-4258
Page 148

PERCH 381750

DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1996-EP2023 19960510. PRIORITY: AT 1995-794 19950511; AT 1995-992 19950612; AT 1996-698 19960417; AT 1996-733 19960423.

GΙ

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. of formula I (R1 = H or ester moiety, R2 = OY, NR4R5, N:R6, Y = H,

alkyl, alkenyl, acyl, carbamoyl, aryl, R4 = H, alkyl, alkenyl, cycloalkyl,

aryl, acyl, heterocyclyl, R5 = H, alkyl, alkenyl, cycloalkyl, aryl, heterocyclyl, C(SR7):NR8, C(NR9R10):Z, CR11:Z, R7 = alkyl or aryl, R8 =

H, cycloalkyl, alkyl, R9 = H or alkyl, R10 = H, alkyl, OH, NH2, Ph, alkenyl, cycloalkyl, aryl, heterocyclyl, N:CHPhe, Phe = aryl, R9 and R10 together with nitrogen form a heterocyclyl, Z = O, S, NR13, R13 = H, alkyl or cycloalkyl, R11 = H, alkyl, aryl, cycloalkyl, or heterocyclyl, R4 and R5 together with nitrogen form a heterocyclyl, R6 = heterocyclyl, Ac = Ac1, COCZ1:CZ2Z3, COCZ1:BDZ4, B = N, CH, Z1 = aryl, cycloalkyl, 1,4-hexadienyl or heterocyclyl, Z2 = H, alkyl, CH2CO2Z5, Z5 = H, alkyl, cycloalkyl, Z3 = H, alkyl, Z4 = H or org. radical, D = O or CH2), were prepd. thereof for

use as pharmaceuticals, i.e. as antibacterial agents. Thus, II was prepd.

via condensation of formylcephemcarboxylic acid deriv. III in 4% aq. MeCN

with guanidine IV in 1-2 N HCl. II has an MHK of 0.01 .mu.g/mL vs. Streptococcus pneumoniae (strain ATCC 49619) compared to 0.02 .mu.g/mL $\,$

for

ceftriaxone.

L3 ANSWER 58 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 184942-58-3 REGISTRY

CN Piperazinium,

4-[[[[7-[[(2-amino-4-thiazolyl)(hydroxyimino)acetyl]amino]-2-carboxy-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]methylene]hydrazino]iminomethyl]-1,1-dimethyl-, chloride, dihydrochloride, [6R-[6.alpha.,7.beta.(Z)]]-(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C20 H27 N10 O5 S2 . 2 Cl H . Cl

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

C1-

PAGE 2-A

2 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:47035 Antibacterial cephalosporins. Ascher, Gerd;
Ludescher, Johannes (Biochemie Gesellschaft Mbh, Austria; Ascher, Gerd;
Ludescher, Johannes). PCT Int. Appl. WO 9635692 A1 19961114, 124 pp.
DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ,

DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS,
LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG,
SI; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB,
GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION:
WO 1996-EP2023 19960510. PRIORITY: AT 1995-794 19950511; AT 1995-992
19950612; AT 1996-698 19960417; AT 1996-733 19960423.

GΙ

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. of formula I (R1 = H or ester moiety, R2 = OY, NR4R5, N:R6, Y = H, alkyl, alkenyl, acyl, carbamoyl, aryl, R4 = H, alkyl, alkenyl, cycloalkyl, Prepared by M. Hale 308-4258 Page 15

aryl, acyl, heterocyclyl, R5 = H, alkyl, alkenyl, cycloalkyl, aryl,
heterocyclyl, C(SR7):NR8, C(NR9R10):Z, CR11:Z, R7 = alkyl or aryl, R8 =

H,

cycloalkyl, alkyl, R9 = H or alkyl, R10 = H, alkyl, OH, NH2, Ph, alkenyl, cycloalkyl, aryl, heterocyclyl, N:CHPhe, Phe = aryl, R9 and R10 together with nitrogen form a heterocyclyl, Z = O, S, NR13, R13 = H, alkyl or cycloalkyl, R11 = H, alkyl, aryl, cycloalkyl, or heterocyclyl, R4 and R5 together with nitrogen form a heterocyclyl, R6 = heterocyclyl, Ac = Acl, COCZ1:CZ2Z3, COCZ1:BDZ4, B = N, CH, Z1 = aryl, cycloalkyl, 1,4-hexadienyl or heterocyclyl, Z2 = H, alkyl, CH2CO2Z5, Z5 = H, alkyl, cycloalkyl, Z3 = H, alkyl, Z4 = H or org. radical, D = O or CH2), were prepd. thereof for use as pharmaceuticals, i.e. as antibacterial agents. Thus, II was

via condensation of formylcephemcarboxylic acid deriv. III in 4% aq. MeCN with guanidine IV in 1-2 N HCl. II has an MHK of 0.01 .mu.g/mL vs. Streptococcus pneumoniae (strain ATCC 49619) compared to 0.02 .mu.g/mL

for

ceftriaxone.

L3 ANSWER 59 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 184942-52-7 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[[(2-amino-4-thiazolyl)(hydroxyimino)acetyl]amino]-3-[[[(4-formyl-1-piperazinyl)iminomethyl]hydrazono]methyl]-8-oxo-, dihydrochloride,
[6R-[6.alpha.,7.beta.(Z)]]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C19 H22 N10 O6 S2 . 2 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry. Double bond geometry as described by E or Z.

● 2 HCl

Prepared by M. Hale 308-4258

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1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)
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REFERENCE 1: 126:47035 Antibacterial cephalosporins. Ascher, Gerd; Ludescher, Johannes (Biochemie Gesellschaft Mbh, Austria; Ascher, Gerd; Ludescher, Johannes). PCT Int. Appl. WO 9635692 A1 19961114, 124 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1996-EP2023 19960510. PRIORITY: AT 1995-794 19950511; AT 1995-992 19950612; AT 1996-698 19960417; AT 1996-733 19960423. GI * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT * Compds. of formula I (R1 = H or ester moiety, R2 = OY, NR4R5, N:R6, Y = AΒ Η, alkyl, alkenyl, acyl, carbamoyl, aryl, R4 = H, alkyl, alkenyl, cycloalkyl, aryl, acyl, heterocyclyl, R5 = H, alkyl, alkenyl, cycloalkyl, aryl, heterocyclyl, C(SR7):NR8, C(NR9R10):Z, CR11:Z, R7 = alkyl or aryl, R8 = Η, cycloalkyl, alkyl, R9 = H or alkyl, R10 = H, alkyl, OH, NH2, Ph, alkenyl, cycloalkyl, aryl, heterocyclyl, N:CHPhe, Phe = aryl, R9 and R10 together with nitrogen form a heterocyclyl, Z = O, S, NR13, R13 = H, alkyl or cycloalkyl, R11 = H, alkyl, aryl, cycloalkyl, or heterocyclyl, R4 and R5 together with nitrogen form a heterocyclyl, R6 = heterocyclyl, Ac = Ac1, COCZ1:CZ2Z3, COCZ1:BDZ4, B = N, CH, Z1 = aryl, cycloalkyl, 1,4-hexadienyl or heterocyclyl, Z2 = H, alkyl, CH2CO2Z5, Z5 = H, alkyl, cycloalkyl, Z3 = H, alkyl, $\overline{Z}4$ = H or org. radical, D = O or CH2), were prepd. thereof for use as pharmaceuticals, i.e. as antibacterial agents. Thus, II was prepd. via condensation of formylcephemcarboxylic acid deriv. III in 4% aq. MeCN with guanidine IV in 1-2 N HCl. II has an MHK of 0.01 .mu.g/mL vs. Streptococcus pneumoniae (strain ATCC 49619) compared to 0.02 .mu.g/mL for ceftriaxone. ANSWER 60 OF 148 REGISTRY COPYRIGHT 2000 ACS L3 RN184942-51-6 REGISTRY CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[(2-amino-4-thiazolyl)(hydroxyimino)acetyl]amino]-3-[[(imino-1piperidinylmethyl)hydrazono]methyl]-8-oxo-, dihydrochloride, [6R-[6.alpha., 7.beta.(Z)]]- (9CI) (CA INDEX NAME) FS STEREOSEARCH MF C19 H23 N9 O5 S2 . 2 Cl H SR CA LC STN Files: CA, CAPLUS

Double bond geometry as described by E or Z.

2 HC1

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:47035 Antibacterial cephalosporins. Ascher, Gerd; Ludescher, Johannes (Biochemie Gesellschaft Mbh, Austria; Ascher, Gerd; Ludescher, Johannes). PCT Int. Appl. WO 9635692 A1 19961114, 124 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ,

DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1996-EP2023 19960510. PRIORITY: AT 1995-794 19950511; AT 1995-992 19950612; AT 1996-698 19960417; AT 1996-733 19960423.

GΙ

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT. *

AB Compds. of formula I (R1 = H or ester moiety, R2 = OY, NR4R5, N:R6, Y = H,

alkyl, alkenyl, acyl, carbamoyl, aryl, R4 = H, alkyl, alkenyl, cycloalkyl,

aryl, acyl, heterocyclyl, R5 = H, alkyl, alkenyl, cycloalkyl, aryl, heterocyclyl, C(SR7):NR8, C(NR9R10):Z, CR11:Z, R7 = alkyl or aryl, R8 =

cycloalkyl, alkyl, R9 = H or alkyl, R10 = H, alkyl, OH, NH2, Ph, alkenyl, cycloalkyl, aryl, heterocyclyl, N:CHPhe, Phe = aryl, R9 and R10 together with nitrogen form a heterocyclyl, Z = O, S, NR13, R13 = H, alkyl or Prepared by M. Hale 308-4258 Page 153

cycloalkyl, R11 = H, alkyl, aryl, cycloalkyl, or heterocyclyl, R4 and R5 together with nitrogen form a heterocyclyl, R6 = heterocyclyl, Ac = Ac1, COCZ1:CZ2Z3, COCZ1:BDZ4, B = N, CH, Z1 = aryl, cycloalkyl, 1,4-hexadienyl or heterocyclyl, Z2 = H, alkyl, CH2CO2Z5, Z5 = H, alkyl, cycloalkyl, Z3 = H, alkyl, Z4 = H or org. radical, D = O or CH2); were prepd. thereof for use as pharmaceuticals, i.e. as antibacterial agents. Thus, II was

via condensation of formylcephemcarboxylic acid deriv. III in 4% aq. MeCN with guanidine IV in 1-2 N HCl. II has an MHK of 0.01 .mu.g/mL vs. Streptococcus pneumoniae (strain ATCC 49619) compared to 0.02 .mu.g/mL

for

ceftriaxone.

L3 ANSWER 61 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 184942-48-1 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

7-[[(2-amino-4-thiazolyl)[(carboxymethoxy)imino]acetyl]amino]-3-[[(imino-1-pyrrolidinylmethyl)hydrazono]methyl]-8-oxo-, dihydrochloride,
[6R-[6.alpha.,7.beta.(Z)]]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C20 H23 N9 O7 S2 . 2 C1 H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry. Double bond geometry as described by E or Z.

● 2 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:47035 Antibacterial cephalosporins. Ascher, Gerd; Ludescher, Johannes (Biochemie Gesellschaft Mbh. Austria; Ascher, Gerd; Prepared by M. Hale 308-4258

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Ludescher, Johannes). PCT Int. Appl. WO 9635692 Al 19961114, 124 pp.
     DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN,
CZ,
     DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS,
     LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG,
     SI; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB,
     GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION:
     WO 1996-EP2023 19960510. PRIORITY: AT 1995-794 19950511; AT 1995-992
     19950612; AT 1996-698 19960417; AT 1996-733 19960423.
GΙ
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
     Compds. of formula I (R1 = H or ester moiety, R2 = OY, NR4R5, N:R6, Y =
Η,
     alkyl, alkenyl, acyl, carbamoyl, aryl, R4 = H, alkyl, alkenyl,
cycloalkyl,
     aryl, acyl, heterocyclyl, R5 = H, alkyl, alkenyl, cycloalkyl, aryl,
     heterocyclyl, C(SR7):NR8, C(NR9R10):Z, CR11:Z, R7 = alkyl or aryl, R8 =
Η,
     cycloalkyl, alkyl, R9 = H or alkyl, R10 = H, alkyl, OH, NH2, Ph, alkenyl,
     cycloalkyl, aryl, heterocyclyl, N:CHPhe, Phe = aryl, R9 and R10 together
     with nitrogen form a heterocyclyl, Z = O, S, NR13, R13 = H, alkyl or
     cycloalkyl, R11 = H, alkyl, aryl, cycloalkyl, or heterocyclyl, R4 and R5
     together with nitrogen form a heterocyclyl, R6 = heterocyclyl, Ac = Ac1,
     COCZ1:CZ2Z3, COCZ1:BDZ4, B = N, CH, Z1 = aryl, cycloalkyl, 1,4-hexadienyl
     or heterocyclyl, Z2 = H, alkyl, CH2CO2Z5, Z5 = H, alkyl, cycloalkyl, Z3 =
     H, alkyl, Z4 = H or org. radical, D = O or CH2), were prepd. thereof for
     use as pharmaceuticals, i.e. as antibacterial agents. Thus, II was
     via condensation of formylcephemcarboxylic acid deriv. III in 4% aq. MeCN
     with guanidine IV in 1-2 N HCl. II has an MHK of 0.01 .mu.g/mL vs.
     Streptococcus pneumoniae (strain ATCC 49619) compared to 0.02 .mu.g/mL
for
     ceftriaxone.
L3
     ANSWER 62 OF 148 REGISTRY COPYRIGHT 2000 ACS
RN
     184942-44-7 REGISTRY
CN
     5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[[(2-amino-4-thiazolyl)[(1-carboxy-1-methylethoxy)imino]acetyl]amino]-3-
     [[(imino-1-pyrrolidinylmethyl)hydrazono]methyl]-8-oxo-, dihydrochloride,
     [6R-[6.alpha.,7.beta.(Z)]]-(9CI) (CA INDEX NAME)
FS
     STEREOSEARCH
     C22 H27 N9 O7 S2 . 2 C1 H
MF
SR
     CA
LC
     STN Files:
                  CA, CAPLUS
Absolute stereochemistry.
```

Double bond geometry as described by E or Z.

● 2 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:47035 Antibacterial cephalosporins. Ascher, Gerd; Ludescher, Johannes (Biochemie Gesellschaft Mbh, Austria; Ascher, Gerd; Ludescher, Johannes). PCT Int. Appl. WO 9635692 A1 19961114, 124 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ,

DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1996-EP2023 19960510. PRIORITY: AT 1995-794 19950511; AT 1995-992 19950612; AT 1996-698 19960417; AT 1996-733 19960423.

GΙ

Η,

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. of formula I (R1 = H or ester moiety, R2 = OY, NR4R5, N:R6, Y = H,

alkyl, alkenyl, acyl, carbamoyl, aryl, R4 = H, alkyl, alkenyl, cycloalkyl,

aryl, acyl, heterocyclyl, R5 = H, alkyl, alkenyl, cycloalkyl, aryl,
heterocyclyl, C(SR7):NR8, C(NR9R10):Z, CR11:Z, R7 = alkyl or aryl, R8 =

cycloalkyl, alkyl, R9 = H or alkyl, R10 = H, alkyl, OH, NH2, Ph, alkenyl, cycloalkyl, aryl, heterocyclyl, N:CHPhe, Phe = aryl, R9 and R10 together with nitrogen form a heterocyclyl, Z = O, S, NR13, R13 = H, alkyl or cycloalkyl, R11 = H, alkyl, aryl, cycloalkyl, or heterocyclyl, R4 and R5 together with nitrogen form a heterocyclyl, R6 = heterocyclyl, Ac = Ac1, COCZ1:CZ2Z3, COCZ1:BDZ4, B = N, CH, Z1 = aryl, cycloalkyl, 1,4-hexadienyl or heterocyclyl, Z2 = H, alkyl, CH2CO2Z5, Z5 = H, alkyl, cycloalkyl, Z3 = Prepared by M. Hale 308-4258

H, alkyl, Z4 = H or org. radical, D = O or CH2), were prepd. thereof for use as pharmaceuticals, i.e. as antibacterial agents. Thus, II was prepd.

via condensation of formylcephemcarboxylic acid deriv. III in 4% aq. MeCN with guanidine IV in 1-2 N HCl. II has an MHK of 0.01 .mu.g/mL vs. Streptococcus pneumoniae (strain ATCC 49619) compared to 0.02 .mu.g/mL

for ceftriaxone.

L3 ANSWER 63 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 184942-33-4 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[[(2Z)-(2-amino-4-thiazolyl) (hydroxyimino)acetyl]amino]-3-[[(imino-1-piperazinylmethyl)hydrazono]methyl]-8-oxo-, trihydrochloride, (6R,7R)-(9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[(2-amino-4-thiazolyl)(hydroxyimino)acetyl]amino]-3-[[(imino-1-piperazinylmethyl)hydrazono]methyl]-8-oxo-, trihydrochloride, [6R-[6.alpha.,7.beta.(Z)]]-

FS STEREOSEARCH

MF C18 H22 N10 O5 S2 . 3 Cl H

SR CA

LC STN Files: CA, CAPLUS

CRN (184943-49-5)

Absolute stereochemistry. Double bond geometry as described by E or Z.

• 3 HCl

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:275783 synthesis of antibacterial substituted Prepared by M. Hale 308-4258

Page 157

 ${\tt acylamino} \, ({\tt methylhydrazono}) \, {\tt methylcephalosporins} \, \, {\tt and} \, \, {\tt intermediates}. \, \\ {\tt Ascher}, \,$

Gerd; Wieser, Josef; Schranz, Michael; Ludescher, Johannes; Hildebrandt, Johannes (Biochemie G.m.b.H., Austria). PCT Int. Appl. WO 9843981 A1 19981008, 46 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-EP1890 19980401. PRIORITY: AT 1997-546 19970401; AT 1997-547 19970401; AT 1997-548 19970401.

GΙ

AB Synthesis of cephalosporins (I) [R1 = H, acyl, carboxyl, alkyl; R2, R3 = H, cycloalkyl, alkyl, alkenyl, alkynyl; R4 = H, C(=Z)R6; R6 = NH2, NHNH2, aminoalkylamino, alkoxy, aryl, cycloaryl, aryloxy, heterocyclyl, alkyl, alkenyl, alkynyl; R5 = H, ester moiety; W = CH, N; V = CH, NO; Z = O, S, NR7; R7 = R2] for use as antibacterials is described. Thus, I (R1 = OCH2F; R2 = Me; R3, R4, R5 = H; W, V = N) is prepd. in 3 steps by acylation of 7-amino-3-formyl-3-cephem-4-carboxylic acid with (5-amino-1,2,4-thiadiazol-3-yl)-(Z)-2-fluoromethoxyiminoacetic acid, reaction of this intermediate with

1-(1-methylhydrazino)iminomethylpiperaz
 ine dihydrochloride followed by chromatog.

REFERENCE 2: 126:47035 Antibacterial cephalosporins. Ascher, Gerd; Ludescher, Johannes (Biochemie Gesellschaft Mbh, Austria; Ascher, Gerd; Ludescher, Johannes). PCT Int. Appl. WO 9635692 A1 19961114, 124 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN,

CZ,

DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1996-EP2023 19960510. PRIORITY: AT 1995-794 19950511; AT 1995-992 19950612; AT 1996-698 19960417; AT 1996-733 19960423.

GΙ

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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
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AB Compds. of formula I (R1 = H or ester moiety, R2 = OY, NR4R5, N:R6, Y = H,

alkyl, alkenyl, acyl, carbamoyl, aryl, R4 = H, alkyl, alkenyl, cycloalkyl,

aryl, acyl, heterocyclyl, R5 = H, alkyl, alkenyl, cycloalkyl, aryl, heterocyclyl, C(SR7):NR8, C(NR9R10):Z, CR11:Z, R7 = alkyl or aryl, R8 =

H, cycloalkyl, alkyl, R9 = H or alkyl, R10 = H, alkyl, OH, NH2, Ph, alkenyl, cycloalkyl, aryl, heterocyclyl, N:CHPhe, Phe = aryl, R9 and R10 together with nitrogen form a heterocyclyl, Z = O, S, NR13, R13 = H, alkyl or cycloalkyl, R11 = H, alkyl, aryl, cycloalkyl, or heterocyclyl, R4 and R5 together with nitrogen form a heterocyclyl, R6 = heterocyclyl, Ac = Ac1, COCZ1:CZ2Z3, COCZ1:BDZ4, B = N, CH, Z1 = aryl, cycloalkyl, 1,4-hexadienyl or heterocyclyl, Z2 = H, alkyl, CH2CO2Z5, Z5 = H, alkyl, cycloalkyl, Z3 = H, alkyl, Z4 = H or org. radical, D = O or CH2), were prepd. thereof for use as pharmaceuticals, i.e. as antibacterial agents. Thus, II was prepd.

via condensation of formylcephemcarboxylic acid deriv. III in 4% aq. MeCN with guanidine IV in 1-2 N HCl. II has an MHK of 0.01 .mu.g/mL vs. Streptococcus pneumoniae (strain ATCC 49619) compared to 0.02 .mu.g/mL

for ceftriaxone.

L3 ANSWER 64 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 184942-18-5 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[(2-amino-4-thiazolyl)(hydroxyimino)acetyl]amino]-3-[[(imino-4-morpholinylmethyl)hydrazono]methyl]-8-oxo-, dihydrochloride, [6R-[6.alpha.,7.beta.(Z)]]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C18 H21 N9 O6 S2 . 2 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

2 HC1

Η,

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:47035 Antibacterial cephalosporins. Ascher, Gerd; Ludescher, Johannes (Biochemie Gesellschaft Mbh, Austria; Ascher, Gerd; Ludescher, Johannes). PCT Int. Appl. WO 9635692 A1 19961114, 124 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN,

CZ,

DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1996-EP2023 19960510. PRIORITY: AT 1995-794 19950511; AT 1995-992 19950612; AT 1996-698 19960417; AT 1996-733 19960423.

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. of formula I (R1 = H or ester moiety, R2 = OY, NR4R5, N:R6, Y = H,

alkyl, alkenyl, acyl, carbamoyl, aryl, R4 = H, alkyl, alkenyl, cycloalkyl,

aryl, acyl, heterocyclyl, R5 = H, alkyl, alkenyl, cycloalkyl, aryl,
heterocyclyl, C(SR7):NR8, C(NR9R10):Z, CR11:Z, R7 = alkyl or aryl, R8 =

cycloalkyl, alkyl, R9 = H or alkyl, R10 = H, alkyl, OH, NH2, Ph, alkenyl, cycloalkyl, aryl, heterocyclyl, N:CHPhe, Phe = aryl, R9 and R10 together with nitrogen form a heterocyclyl, Z = O, S, NR13, R13 = H, alkyl or cycloalkyl, R11 = H, alkyl, aryl, cycloalkyl, or heterocyclyl, R4 and R5 together with nitrogen form a heterocyclyl, R6 = heterocyclyl, Ac = Ac1, COCZ1:CZ2Z3, COCZ1:BDZ4, B = N, CH, Z1 = aryl, cycloalkyl, 1,4-hexadienyl Prepared by M. Hale 308-4258

or heterocyclyl, Z2 = H, alkyl, CH2CO2Z5, Z5 = H, alkyl, cycloalkyl, Z3 = H, alkyl, Z4 = H or org. radical, D = O or CH2), were prepd. thereof for use as pharmaceuticals, i.e. as antibacterial agents. Thus, II was prepd.

via condensation of formylcephemcarboxylic acid deriv. III in 4% aq. MeCN with guanidine IV in 1-2 N HCl. II has an MHK of 0.01 .mu.g/mL vs. Streptococcus pneumoniae (strain ATCC 49619) compared to 0.02 .mu.g/mL

for

ceftriaxone.

L3 ANSWER 65 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 184942-10-7 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[(2-amino-4-thiazolyl)(hydroxyimino)acetyl]amino]-3-[[[(ethylamino)-1-pyrrolidinylmethylene]hydrazono]methyl]-8-oxo-, dihydrochloride, [6R-[6.alpha.,7.beta.(Z)]]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C20 H25 N9 O5 S2 . 2 C1 H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry. Double bond geometry as described by E or Z.

● 2 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:47035 Antibacterial cephalosporins. Ascher, Gerd; Ludescher, Johannes (Biochemie Gesellschaft Mbh, Austria; Ascher, Gerd; Ludescher, Johannes). PCT Int. Appl. WO 9635692 A1 19961114, 124 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ,

DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, Prepared by M. Hale 308-4258

SI; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1996-EP2023 19960510. PRIORITY: AT 1995-794 19950511; AT 1995-992 19950612; AT 1996-698 19960417; AT 1996-733 19960423.

GΙ

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. of formula I (R1 = H or ester moiety, R2 = OY, NR4R5, N:R6, Y = H,

alkyl, alkenyl, acyl, carbamoyl, aryl, R4 = H, alkyl, alkenyl, cycloalkyl,

aryl, acyl, heterocyclyl, R5 = H, alkyl, alkenyl, cycloalkyl, aryl, heterocyclyl, C(SR7):NR8, C(NR9R10):Z, CR11:Z, R7 = alkyl or aryl, R8 =

Η,

cycloalkyl, alkyl, R9 = H or alkyl, R10 = H, alkyl, OH, NH2, Ph, alkenyl, cycloalkyl, aryl, heterocyclyl, N:CHPhe, Phe = aryl, R9 and R10 together with nitrogen form a heterocyclyl, Z = O, S, NR13, R13 = H, alkyl or cycloalkyl, R11 = H, alkyl, aryl, cycloalkyl, or heterocyclyl, R4 and R5 together with nitrogen form a heterocyclyl, R6 = heterocyclyl, Ac = Ac1, COCZ1:CZ2Z3, COCZ1:BDZ4, B = N, CH, Z1 = aryl, cycloalkyl, 1,4-hexadienyl or heterocyclyl, Z2 = H, alkyl, CH2CO2Z5, Z5 = H, alkyl, cycloalkyl, Z3 = H, alkyl, Z4 = H or org. radical, D = O or CH2), were prepd. thereof for use as pharmaceuticals, i.e. as antibacterial agents. Thus, II was prepd.

via condensation of formylcephemcarboxylic acid deriv. III in 4% aq. MeCN with guanidine IV in 1-2 N HCl. II has an MHK of 0.01 .mu.g/mL vs. Streptococcus pneumoniae (strain ATCC 49619) compared to 0.02 .mu.g/mL

for

ceftriaxone.

- L3 ANSWER 66 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 184942-04-9 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[(2-amino-4-thiazolyl)(methoxyimino)acetyl]amino]-3-[[[(4-formyl-1-piperazinyl)iminomethyl]methylhydrazono]methyl]-8-oxo-, dihydrochloride, [6R-[6.alpha.,7.beta.(Z)]]- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C21 H26 N10 O6 S2 . 2 Cl H
- SR CA
- LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

2 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:47035 Antibacterial cephalosporins. Ascher, Gerd; Ludescher, Johannes (Biochemie Gesellschaft Mbh, Austria; Ascher, Gerd; Ludescher, Johannes). PCT Int. Appl. WO 9635692 A1 19961114, 124 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN,

CZ,

DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1996-EP2023 19960510. PRIORITY: AT 1995-794 19950511; AT 1995-992 19950612; AT 1996-698 19960417; AT 1996-733 19960423.

Η,

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. of formula I (R1 = H or ester moiety, R2 = OY, NR4R5, N:R6, Y = H,

alkyl, alkenyl, acyl, carbamoyl, aryl, R4 = H, alkyl, alkenyl, cycloalkyl,

aryl, acyl, heterocyclyl, R5 = H, alkyl, alkenyl, cycloalkyl, aryl,
heterocyclyl, C(SR7):NR8, C(NR9R10):Z, CR11:Z, R7 = alkyl or aryl, R8 =

cycloalkyl, alkyl, R9 = H or alkyl, R10 = H, alkyl, OH, NH2, Ph, alkenyl, cycloalkyl, aryl, heterocyclyl, N:CHPhe, Phe = aryl, R9 and R10 together with nitrogen form a heterocyclyl, Z = O, S, NR13, R13 = H, alkyl or cycloalkyl, R11 = H, alkyl, aryl, cycloalkyl, or heterocyclyl, R4 and R5 together with nitrogen form a heterocyclyl, R6 = heterocyclyl, Ac = Ac1, COCZ1:CZ2Z3, COCZ1:BDZ4, B = N, CH, Z1 = aryl, cycloalkyl, 1,4-hexadienyl Prepared by M. Hale 308-4258

or heterocyclyl, Z2 = H, alkyl, CH2CO2Z5, Z5 = H, alkyl, cycloalkyl, Z3 = H, alkyl, Z4 = H or org. radical, D = O or CH2), were prepd. thereof for use as pharmaceuticals, i.e. as antibacterial agents. Thus, II was prepd.

via condensation of formylcephemcarboxylic acid deriv. III in 4% aq. MeCN with guanidine IV in 1-2 N HCl. II has an MHK of 0.01 .mu.g/mL vs. Streptococcus pneumoniae (strain ATCC 49619) compared to 0.02 .mu.g/mL

for

ceftriaxone.

L3 ANSWER 67 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 184942-03-8 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[[(2-amino-4-thiazolyl)(methoxyimino)acetyl]amino]-3-[[(imino-1-piperazinylmethyl)methylhydrazono]methyl]-8-oxo-, trihydrochloride,
[6R-[6.alpha.,7.beta.(Z)]]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C20 H26 N10 O5 S2 . 3 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

• 3 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:47035 Antibacterial cephalosporins. Ascher, Gerd;
Ludescher, Johannes (Biochemie Gesellschaft Mbh, Austria; Ascher, Gerd;
Ludescher, Johannes). PCT Int. Appl. WO 9635692 Al 19961114, 124 pp.
DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN,
CZ,
DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS,
Prepared by M. Halé 308-4258

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GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION:
     WO 1996-EP2023 19960510. PRIORITY: AT 1995-794 19950511; AT 1995-992
     19950612; AT 1996-698 19960417; AT 1996-733 19960423.
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
     Compds. of formula I (R1 = H or ester moiety, R2 = OY, NR4R5, N:R6, Y =
     alkyl, alkenyl, acyl, carbamoyl, aryl, R4 = H, alkyl, alkenyl,
cycloalkyl,
     aryl, acyl, heterocyclyl, R5 = H, alkyl, alkenyl, cycloalkyl, aryl,
     heterocyclyl, C(SR7):NR8, C(NR9R10):Z, CR11:Z, R7 = alkyl or aryl, R8 =
     cycloalkyl, alkyl, R9 = H or alkyl, R10 = H, alkyl, OH, NH2, Ph, alkenyl,
     cycloalkyl, aryl, heterocyclyl, N:CHPhe, Phe = aryl, R9 and R10 together
     with nitrogen form a heterocyclyl, Z = O, S, NR13, R13 = H, alkyl or
     cycloalkyl, R11 = H, alkyl, aryl, cycloalkyl, or heterocyclyl, R4 and R5
     together with nitrogen form a heterocyclyl, R6 = heterocyclyl, Ac = Ac1,
     COCZ1:CZ2Z3, COCZ1:BDZ4, B = N, CH, Z1 = aryl, cycloalkyl, 1,4-hexadienyl
     or heterocyclyl, Z2 = H, alkyl, CH2CO2Z5, Z5 = H, alkyl, cycloalkyl, Z3 =
     H, alkyl, Z4 = H or org. radical, D = O or CH2), were prepd. thereof for
     use as pharmaceuticals, i.e. as antibacterial agents. Thus, II was
prepd.
     via condensation of formylcephemcarboxylic acid deriv. III in 4% aq. MeCN
     with guanidine IV in 1-2 N HCl. II has an MHK of 0.01 .mu.g/mL vs.
     Streptococcus pneumoniae (strain ATCC 49619) compared to 0.02 .mu.g/mL
     ceftriaxone.
     ANSWER 68 OF 148 REGISTRY COPYRIGHT 2000 ACS
     184941-99-9 REGISTRY
     Piperazinium,
4-[[[[7-[[(2-amino-4-thiazolyl)(methoxyimino)acetyl]amino]-2-
     carboxy-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-
     yl]methylene]hydrazino]iminomethyl]-1,1-dimethyl-, chloride,
     dihydrochloride, [6R-[6.alpha.,7.beta.(Z)]]- (9CI) (CA INDEX NAME)
     STEREOSEARCH
     C21 H29 N10 O5 S2 . 2 Cl H . Cl
                  CA, CAPLUS
     STN Files:
```

LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB,

GΙ

AB Η,

Η,

for

L3RN

CN

FS

MF

SR LC

Absolute stereochemistry.

Double bond geometry as described by E or Z.

• Cl-

PAGE 2-A

2 HC1

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:47035 Antibacterial cephalosporins. Ascher, Gerd;
Ludescher, Johannes (Biochemie Gesellschaft Mbh, Austria; Ascher, Gerd;
Ludescher, Johannes). PCT Int. Appl. WO 9635692 Al 19961114, 124 pp.
DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN,
CZ,

DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS,
LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG,
SI; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB,
GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION:
WO 1996-EP2023 19960510. PRIORITY: AT 1995-794 19950511; AT 1995-992
19950612; AT 1996-698 19960417; AT 1996-733 19960423.

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. of formula I (R1 = H or ester moiety, R2 = OY, NR4R5, N:R6, Y = H, alkyl, alkenyl, acyl carbamoyl, aryl, R4 = H, alkyl, alkenyl, cycloalkyl, Prepared by M. Haie 308-4258 Page 16

aryl, acyl, heterocyclyl, R5 = H, alkyl, alkenyl, cycloalkyl, aryl, heterocyclyl, C(SR7):NR8, C(NR9R10):Z, CR11:Z, R7 = alkyl or aryl, R8 =

Η, cycloalkyl, alkyl, R9 = H or alkyl, R10 = H, alkyl, OH, NH2, Ph, alkenyl, cycloalkyl, aryl, heterocyclyl, N:CHPhe, Phe = aryl, R9 and R10 together with nitrogen form a heterocyclyl, Z = O, S, NR13, R13 = H, alkyl or cycloalkyl, R11 = H, alkyl, aryl, cycloalkyl, or heterocyclyl, R4 and R5 together with nitrogen form a heterocyclyl, R6 = heterocyclyl, Ac = Ac1, COCZ1:CZ2Z3, COCZ1:BDZ4, B = N, CH, Z1 = aryl, cycloalkyl, 1,4-hexadienyl or heterocyclyl, Z2 = H, alkyl, CH2CO2Z5, Z5 = H, alkyl, cycloalkyl, Z3 = H, alkyl, Z4 = H or org. radical, D = O or CH2), were prepd. thereof for use as pharmaceuticals, i.e. as antibacterial agents. Thus, II was prepd.

via condensation of formylcephemcarboxylic acid deriv. III in 4% aq. MeCN with guanidine IV in 1-2 N HCl. II has an MHK of 0.01 .mu.g/mL vs. Streptococcus pneumoniae (strain ATCC 49619) compared to 0.02 .mu.g/mL

for ceftriaxone.

L3 ANSWER 69 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 184941-87-5 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[(2-amino-4-thiazolyl)(methoxyimino)acetyl]amino]-3-[[((4-formyl-1piperazinyl) (methylamino) methylene] hydrazono] methyl] -8-oxo-, dihydrochloride, [6R-[6.alpha.,7.beta.(Z)]]- (9CI) (CA INDEX NAME) FS

STEREOSEARCH

MF C21 H26 N10 O6 S2 . 2 Cl H

SR

LC STN Files: CA, CAPLUS

Absolute stereochemistry. Double bond geometry as described by E or Z.

2 HCl

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1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)
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REFERENCE 1: 126:47035 Antibacterial cephalosporins. Ascher, Gerd;
     Ludescher, Johannes (Biochemie Gesellschaft Mbh, Austria; Ascher, Gerd;
     Ludescher, Johannes). PCT Int. Appl. WO 9635692 Al 19961114, 124 pp.
     DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN,
CZ,
    DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS,
    LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG,
    SI; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB,
    GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION:
    WO 1996-EP2023 19960510. PRIORITY: AT 1995-794 19950511; AT 1995-992
     19950612; AT 1996-698 19960417; AT 1996-733 19960423.
GI
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
AΒ
    Compds. of formula I (R1 = H or ester moiety, R2 = OY, NR4R5, N:R6, Y =
Η,
     alkyl, alkenyl, acyl, carbamoyl, aryl, R4 = H, alkyl, alkenyl,
     aryl, acyl, heterocyclyl, R5 = H, alkyl, alkenyl, cycloalkyl, aryl,
    heterocyclyl, C(SR7):NR8, C(NR9R10):Z, CR11:Z, R7 = alkyl or aryl, R8 =
Η,
    cycloalkyl, alkyl, R9 = H or alkyl, R10 = H, alkyl, OH, NH2, Ph, alkenyl,
    cycloalkyl, aryl, heterocyclyl, N:CHPhe, Phe = aryl, R9 and R10 together
    with nitrogen form a heterocyclyl, Z = O, S, NR13, R13 = H, alkyl or
    cycloalkyl, R11 = H, alkyl, aryl, cycloalkyl, or heterocyclyl, R4 and R5
    together with nitrogen form a heterocyclyl, R6 = heterocyclyl, Ac = Ac1,
    COCZ1:CZ2Z3, COCZ1:BDZ4, B = N, CH, Z1 = aryl, cycloalkyl, 1,4-hexadienyl
    or heterocyclyl, Z2 = H, alkyl, CH2CO2Z5, Z5 = H, alkyl, cycloalkyl, Z3 =
    H, alkyl, Z4 = H or org. radical, D = O or CH2), were prepd. thereof for
    use as pharmaceuticals, i.e. as antibacterial agents. Thus, II was
prepd.
     via condensation of formylcephemcarboxylic acid deriv. III in 4% aq. MeCN
    with guanidine IV in 1-2 N HCl. II has an MHK of 0.01 .mu.g/mL vs.
     Streptococcus pneumoniae (strain ATCC 49619) compared to 0.02 .mu.g/mL
for
    ceftriaxone.
    ANSWER 70 OF 148 REGISTRY COPYRIGHT 2000 ACS
L3
    184941-83-1 REGISTRY
RN
     5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
CN
    7-[[(2-amino-4-thiazolyl)(methoxyimino)acetyl]amino]-3-[[(imino-1-
    piperazinylmethyl)hydrazono]methyl]-8-oxo-, trihydrochloride,
     [6R-[6.alpha.,7.beta.(Z)]]- (9CI) (CA INDEX NAME)
FS
     STEREOSEARCH
    C19 H24 N10 O5 S2 . 3 Cl H
ΜF
SR
    CA
LC
     STN Files:
                 CA, CAPLUS
```

Double bond geometry as described by E or Z.

• 3 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

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Ludescher, Johannes (Biochemie Gesellschaft Mbh, Austria; Ascher, Gerd;
Ludescher, Johannes). PCT Int. Appl. WO 9635692 A1 19961114, 124 pp.
DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN,
CZ,

DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS,
LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG,
SI; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB,
GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION:
WO 1996-EP2023 19960510. PRIORITY: AT 1995-794 19950511; AT 1995-992
19950612; AT 1996-698 19960417; AT 1996-733 19960423.

GΙ

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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. of formula I (R1 = H or ester moiety, R2 = OY, NR4R5, N:R6, Y = H,

alkyl, alkenyl, acyl, carbamoyl, aryl, R4 = H, alkyl, alkenyl, cycloalkyl,

aryl, acyl, heterocyclyl, R5 = H, alkyl, alkenyl, cycloalkyl, aryl, heterocyclyl, C(SR7):NR8, C(NR9R10):Z, CR11:Z, R7 = alkyl or aryl, R8 =

cycloalkyl, alkyl, R9 = H or alkyl, R10 = H, alkyl, OH, NH2, Ph, alkenyl, cycloalkyl, aryl, heterocyclyl, N:CHPhe, Phe = aryl, R9 and R10 together with nitrogen form a heterocyclyl, Z = O, S, NR13, R13 = H, alkyl or Prepared by M. Hale 308-4258

cycloalkyl, R11 = H, alkyl, aryl, cycloalkyl, or heterocyclyl, R4 and R5 together with nitrogen form a heterocyclyl, R6 = heterocyclyl, Ac = Ac1, COCZ1:CZ2Z3, COCZ1:BDZ4, B = N, CH, Z1 = aryl, cycloalkyl, 1,4-hexadienyl or heterocyclyl, Z2 = H, alkyl, CH2CO2Z5, Z5 = H, alkyl, cycloalkyl, Z3 = H, alkyl, Z4 = H or org. radical, D = O or CH2), were prepd. thereof for use as pharmaceuticals, i.e. as antibacterial agents. Thus, II was prepd.

via condensation of formylcephemcarboxylic acid deriv. III in 4% aq. MeCN with guanidine IV in 1-2 N HCl. II has an MHK of 0.01 .mu.g/mL vs. Streptococcus pneumoniae (strain ATCC 49619) compared to 0.02 .mu.g/mL

for

ceftriaxone.

L3 ANSWER 71 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 184941-82-0 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[(2-amino-4-thiazolyl)(methoxyimino)acetyl]amino]-3-[[(imino-1-piperidinylmethyl)hydrazono]methyl]-8-oxo-, dihydrochloride, [6R-[6.alpha.,7.beta.(Z)]]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C20 H25 N9 O5 S2 . 2 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

● 2 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:47035 Antibacterial cephalosporins. Ascher, Gerd; Ludescher, Johannes (Biochemie Gesellschaft Mbh, Austria; Ascher, Gerd; Ludescher, Johannes). PCT Int. Appl. WO 9635692 A1 19961114, 124 pp. Prepared by M. Hale 308-4258

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DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN,
CZ,
     DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS,
     LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG,
     SI; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB,
     GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION:
     WO 1996-EP2023 19960510. PRIORITY: AT 1995-794 19950511; AT 1995-992
     19950612; AT 1996-698 19960417; AT 1996-733 19960423.
GI
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
AB
     Compds. of formula I (R1 = H or ester moiety, R2 = OY, NR4R5, N:R6, Y =
Η,
     alkyl, alkenyl, acyl, carbamoyl, aryl, R4 = H, alkyl, alkenyl,
     aryl, acyl, heterocyclyl, R5 = H, alkyl, alkenyl, cycloalkyl, aryl,
     heterocyclyl, C(SR7):NR8, C(NR9R10):Z, CR11:Z, R7 = alkyl or aryl, R8 =
Η,
     cycloalkyl, alkyl, R9 = H or alkyl, R10 = H, alkyl, OH, NH2, Ph, alkenyl,
     cycloalkyl, aryl, heterocyclyl, N:CHPhe, Phe = aryl, R9 and R10 together
     with nitrogen form a heterocyclyl, Z = O, S, NR13, R13 = H, alkyl or
     cycloalkyl, R11 = H, alkyl, aryl, cycloalkyl, or heterocyclyl, R4 and R5
     together with nitrogen form a heterocyclyl, R6 = heterocyclyl, Ac = Ac1,
     COCZ1:CZ2Z3, COCZ1:BDZ4, B = N, CH, Z1 = aryl, cycloalkyl, 1,4-hexadienyl
     or heterocyclyl, Z2 = H, alkyl, CH2CO2Z5, Z5 = H, alkyl, cycloalkyl, Z3 =
     H, alkyl, Z4 = H or org. radical, D = O or CH2), were prepd. thereof for
     use as pharmaceuticals, i.e. as antibacterial agents. Thus, II was
prepd.
     via condensation of formylcephemcarboxylic acid deriv. III in 4% aq. MeCN
     with guanidine IV in 1-2 N HCl. II has an MHK of 0.01 .mu.g/mL vs.
     Streptococcus pneumoniae (strain ATCC 49619) compared to 0.02 .mu.g/mL
for
     ceftriaxone.
L3
     ANSWER 72 OF 148 REGISTRY COPYRIGHT 2000 ACS
RN
     184941-79-5 REGISTRY
     5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
CN
7-[[(2-amino-4-thiazolyl)(methoxyimino)acetyl]amino]-3-[[(methylamino)-1-
     piperazinylmethylene]hydrazono]methyl]-8-oxo-, trihydrochloride,
     [6R-[6.alpha., 7.beta.(Z)]]- (9CI) (CA INDEX NAME)
FS
     STEREOSEARCH
     C20 H26 N10 O5 S2 . 3 Cl H
MF
SR
     CA
LC
     STN Files:
                  CA, CAPLUS
```

Absolute stereochemistry.

Double bond geometry as described by E or Z.

3 HC1

1 REFERENCES IN FILE CA (1967 TO DATE)
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CZ,

DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1996-EP2023 19960510. PRIORITY: AT 1995-794 19950511; AT 1995-992 19950612; AT 1996-698 19960417; AT 1996-733 19960423.

GΙ

Η,

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. of formula I (R1 = H or ester moiety, R2 = OY, NR4R5, N:R6, Y = H,

alkyl, alkenyl, acyl, carbamoyl, aryl, R4 = H, alkyl, alkenyl,
cycloalkyl,

aryl, acyl, heterocyclyl, R5 = H, alkyl, alkenyl, cycloalkyl, aryl,
heterocyclyl, C(SR7):NR8, C(NR9R10):Z, CR11:Z, R7 = alkyl or aryl, R8 =

cycloalkyl, alkyl, R9 = H or alkyl, R10 = H, alkyl, OH, NH2, Ph, alkenyl, cycloalkyl, aryl, heterocyclyl, N:CHPhe, Phe = aryl, R9 and R10 together with nitrogen form a heterocyclyl, Z = O, S, NR13, R13 = H, alkyl or cycloalkyl, R11 = H, alkyl, aryl, cycloalkyl, or heterocyclyl, R4 and R5 together with nitrogen form a heterocyclyl, R6 = heterocyclyl, Ac = Acl, COCZ1:CZ2Z3, COCZ1:BDZ4, B = N, CH, Z1 = aryl, cycloalkyl, 1,4-hexadienyl Prepared by M. Hale 308-4258

or heterocyclyl, Z2 = H, alkyl, CH2CO2Z5, Z5 = H, alkyl, cycloalkyl, Z3 = H, alkyl, Z4 = H or org. radical, D = O or CH2), were prepd. thereof for use as pharmaceuticals, i.e. as antibacterial agents. Thus, II was prepd.

via condensation of formylcephemcarboxylic acid deriv. III in 4% aq. MeCN with guanidine IV in 1-2 N HCl. II has an MHK of 0.01 .mu.g/mL vs. Streptococcus pneumoniae (strain ATCC 49619) compared to 0.02 .mu.g/mL

for ceftriaxone.

L3 ANSWER 73 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 184941-70-6 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[(2-amino-4-thiazolyl) (methoxyimino)acetyl]amino]-3-[[(imino-4-morpholinylmethyl)hydrazono]methyl]-8-oxo-, dihydrochloride, [6R-[6.alpha.,7.beta.(Z)]]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C19 H23 N9 O6 S2 . 2 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry. Double bond geometry as described by E or Z.

• 2 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:47035 Antibacterial cephalosporins. Ascher, Gerd;
Ludescher, Johannes (Biochemie Gesellschaft Mbh, Austria; Ascher, Gerd;
Ludescher, Johannes). PCT Int. Appl. WO 9635692 Al 19961114, 124 pp.
DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN,
CZ,

DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, Prepared by M. Hale 308-4258

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SI; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB,
     GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION:
    WO 1996-EP2023 19960510. PRIORITY: AT 1995-794 19950511; AT 1995-992
     19950612; AT 1996-698 19960417; AT 1996-733 19960423.
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
     Compds. of formula I (R1 = H or ester moiety, R2 = OY, NR4R5, N:R6, Y =
     alkyl, alkenyl, acyl, carbamoyl, aryl, R4 = H, alkyl, alkenyl,
cycloalkyl,
     aryl, acyl, heterocyclyl, R5 = H, alkyl, alkenyl, cycloalkyl, aryl,
    heterocyclyl, C(SR7):NR8, C(NR9R10):Z, CR11:Z, R7 = alkyl or aryl, R8 =
     cycloalkyl, alkyl, R9 = H or alkyl, R10 = H, alkyl, OH, NH2, Ph, alkenyl,
     cycloalkyl, aryl, heterocyclyl, N:CHPhe, Phe = aryl, R9 and R10 together
     with nitrogen form a heterocyclyl, Z = O, S, NR13, R13 = H, alkyl or
     cycloalkyl, R11 = H, alkyl, aryl, cycloalkyl, or heterocyclyl, R4 and R5
     together with nitrogen form a heterocyclyl, R6 = heterocyclyl, Ac = Ac1,
    COCZ1:CZ2Z3, COCZ1:BDZ4, B = N, CH, Z1 = aryl, cycloalkyl, 1,4-hexadienyl
     or heterocyclyl, Z2 = H, alkyl, CH2CO2Z5, Z5 = H, alkyl, cycloalkyl, Z3 =
     H, alkyl, Z4 = H or org. radical, D = O or CH2), were prepd. thereof for
    use as pharmaceuticals, i.e. as antibacterial agents. Thus, II was
     via condensation of formylcephemcarboxylic acid deriv. III in 4% aq. MeCN
     with quanidine IV in 1-2 N HCl. II has an MHK of 0.01 .mu.g/mL vs.
     Streptococcus pneumoniae (strain ATCC 49619) compared to 0.02 .mu.g/mL
     ceftriaxone.
    ANSWER 74 OF 148 REGISTRY COPYRIGHT 2000 ACS
     184941-66-0 REGISTRY
     5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[((2-amino-4-thiazolyl)(methoxyimino)acetyl]amino]-3-[[((methylamino)-4-
     morpholinylmethylene]hydrazono]methyl]-8-oxo-, dihydrochloride,
     [6R-[6.alpha., 7.beta.(Z)]]- (9CI) (CA INDEX NAME)
     STEREOSEARCH
    C20 H25 N9 O6 S2 . 2 Cl H
    CA
```

LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG,

GΙ

AB Η,

Η,

for

L3 RN

CN

FS

MFSR

LC

STN Files:

Absolute stereochemistry.

CA, CAPLUS

Double bond geometry as described by E or Z.

2 HC1

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:47035 Antibacterial cephalosporins. Ascher, Gerd; Ludescher, Johannes (Biochemie Gesellschaft Mbh, Austria; Ascher, Gerd; Ludescher, Johannes). PCT Int. Appl. WO 9635692 Al 19961114, 124 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN,

CZ,

DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1996-EP2023 19960510. PRIORITY: AT 1995-794 19950511; AT 1995-992 19950612; AT 1996-698 19960417; AT 1996-733 19960423.

GI

Η,

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. of formula I (R1 = H or ester moiety, R2 = OY, NR4R5, N:R6, Y = H,

alkyl, alkenyl, acyl, carbamoyl, aryl, R4 = H, alkyl, alkenyl,
cycloalkyl,

aryl, acyl, heterocyclyl, R5 = H, alkyl, alkenyl, cycloalkyl, aryl,
heterocyclyl, C(SR7):NR8, C(NR9R10):Z, CR11:Z, R7 = alkyl or aryl, R8 =

cycloalkyl, alkyl, R9 = H or alkyl, R10 = H, alkyl, OH, NH2, Ph, alkenyl, cycloalkyl, aryl, heterocyclyl, N:CHPhe, Phe = aryl, R9 and R10 together with nitrogen form a heterocyclyl, Z = O, S, NR13, R13 = H, alkyl or cycloalkyl, R11 = H, alkyl, aryl, cycloalkyl, or heterocyclyl, R4 and R5 together with nitrogen form a heterocyclyl, R6 = heterocyclyl, Ac = Acl, COCZ1:CZ2Z3, COCZ1:BDZ4, B = N, CH, Z1 = aryl, cycloalkyl, 1,4-hexadienyl Prepared by M. Hale 308-4258

or heterocyclyl, Z2 = H, alkyl, CH2CO2Z5, Z5 = H, alkyl, cycloalkyl, Z3 = H, alkyl, Z4 = H or org. radical, D = O or CH2), were prepd. thereof for use as pharmaceuticals, i.e. as antibacterial agents. Thus, II was prepd.

via condensation of formylcephemcarboxylic acid deriv. III in 4% aq. MeCN with guanidine IV in 1-2 N HCl. II has an MHK of 0.01 .mu.g/mL vs. Streptococcus pneumoniae (strain ATCC 49619) compared to 0.02 .mu.g/mL

for or

ceftriaxone.

L3 ANSWER 75 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 184941-47-7 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[(2-amino-4-thiazolyl)(hydroxyimino)acetyl]amino]-3-[[(imino-1-pyrrolidinylmethyl)hydrazono]methyl]-8-oxo-, dihydrochloride, [6R-[6.alpha.,7.beta.(Z)]]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C18 H21 N9 O5 S2 . 2 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

• 2 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:47035 Antibacterial cephalosporins. Ascher, Gerd; Ludescher, Johannes (Biochemie Gesellschaft Mbh, Austria; Ascher, Gerd; Ludescher, Johannes). PCT Int. Appl. WO 9635692 A1 19961114, 124 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ.

DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, Prepared by M. Hale 308-4258

SI; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1996-EP2023 19960510. PRIORITY: AT 1995-794 19950511; AT 1995-992 19950612; AT 1996-698 19960417; AT 1996-733 19960423.

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. of formula I (R1 = H or ester moiety, R2 = OY, NR4R5, N:R6, Y = H,

alkyl, alkenyl, acyl, carbamoyl, aryl, R4 = H, alkyl, alkenyl,
cycloalkyl,

aryl, acyl, heterocyclyl, R5 = H, alkyl, alkenyl, cycloalkyl, aryl, heterocyclyl, C(SR7):NR8, C(NR9R10):Z, CR11:Z, R7 = alkyl or aryl, R8 =

H, cycloalkyl, alkyl, R9 = H or alkyl, R10 = H, alkyl, OH, NH2, Ph, alkenyl, cycloalkyl, aryl, heterocyclyl, N:CHPhe, Phe = aryl, R9 and R10 together with nitrogen form a heterocyclyl, Z = O, S, NR13, R13 = H, alkyl or cycloalkyl, R11 = H, alkyl, aryl, cycloalkyl, or heterocyclyl, R4 and R5 together with nitrogen form a heterocyclyl, R6 = heterocyclyl, Ac = Ac1, COCZ1:CZ2Z3, COCZ1:BDZ4, B = N, CH, Z1 = aryl, cycloalkyl, 1,4-hexadienyl or heterocyclyl, Z2 = H, alkyl, CH2CO2Z5, Z5 = H, alkyl, cycloalkyl, Z3 = H, alkyl, Z4 = H or org. radical, D = O or CH2), were prepd. thereof for use as pharmaceuticals, i.e. as antibacterial agents. Thus, II was prepd.

via condensation of formylcephemcarboxylic acid deriv. III in 4% aq. MeCN with guanidine IV in 1-2 N HCl. II has an MHK of 0.01 .mu.g/mL vs. Streptococcus pneumoniae (strain ATCC 49619) compared to 0.02 .mu.g/mL

for

ceftriaxone.

L3 ANSWER 76 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 184941-43-3 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[(2-amino-4-thiazolyl)(methoxyimino)acetyl]amino]-3-[[[(ethylamino)-1-pyrrolidinylmethylene]hydrazono]methyl]-8-oxo-, dihydrochloride, [6R-[6.alpha.,7.beta.(Z)]]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C21 H27 N9 O5 S2 . 2 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry. Double bond geometry as described by E or Z.

● 2 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:47035 Antibacterial cephalosporins. Ascher, Gerd; Ludescher, Johannes (Biochemie Gesellschaft Mbh, Austria; Ascher, Gerd; Ludescher, Johannes). PCT Int. Appl. WO 9635692 A1 19961114, 124 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN,

CZ,

DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1996-EP2023 19960510. PRIORITY: AT 1995-794 19950511; AT 1995-992 19950612; AT 1996-698 19960417; AT 1996-733 19960423.

GΙ

Η,

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. of formula I (R1 = H or ester moiety, R2 = OY, NR4R5, N:R6, Y = H,

alkyl, alkenyl, acyl, carbamoyl, aryl, R4 = H, alkyl, alkenyl, cycloalkyl,

aryl, acyl, heterocyclyl, R5 = H, alkyl, alkenyl, cycloalkyl, aryl,
heterocyclyl, C(SR7):NR8, C(NR9R10):Z, CR11:Z, R7 = alkyl or aryl, R8 =

cycloalkyl, alkyl, R9 = H or alkyl, R10 = H, alkyl, OH, NH2, Ph, alkenyl, cycloalkyl, aryl, heterocyclyl, N:CHPhe, Phe = aryl, R9 and R10 together with nitrogen form a heterocyclyl, Z = O, S, NR13, R13 = H, alkyl or cycloalkyl, R11 = H, alkyl, aryl, cycloalkyl, or heterocyclyl, R4 and R5 together with nitrogen form a heterocyclyl, R6 = heterocyclyl, Ac = Ac1, COCZ1:CZ2Z3, COCZ1:BDZ4, B = N, CH, Z1 = aryl, cycloalkyl, 1,4-hexadienyl or heterocyclyl, Z2 = H, alkyl, CH2CO2Z5, Z5 = H, alkyl, cycloalkyl, Z3 = Prepared by M. Hale 308-4258

H, alkyl, Z4 = H or org. radical, D = O or CH2), were prepd. thereof for use as pharmaceuticals, i.e. as antibacterial agents. Thus, II was prepd.

via condensation of formylcephemcarboxylic acid deriv. III in 4% aq. MeCN with guanidine IV in 1-2 N HCl. II has an MHK of 0.01 .mu.g/mL vs. Streptococcus pneumoniae (strain ATCC 49619) compared to 0.02 .mu.g/mL

for

ceftriaxone.

L3 ANSWER 77 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 184941-39-7 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[(2-amino-4-thiazolyl)(methoxyimino)acetyl]amino]-3-[[(imino-1-pyrrolidinylmethyl)hydrazono]methyl]-8-oxo-, dihydrochloride, [6R-[6.alpha.,7.beta.(Z)]]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C19 H23 N9 O5 S2 . 2 Cl H

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as described by E or Z.

● 2 HCl

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:47035 Antibacterial cephalosporins. Ascher, Gerd; Ludescher, Johannes (Biochemie Gesellschaft Mbh, Austria; Ascher, Gerd; Ludescher, Johannes). PCT Int. Appl. WO 9635692 A1 19961114, 124 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN,

CZ,

DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, Prepared by M. Hale 308-4258

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WO 1996-EP2023 19960510. PRIORITY: AT 1995-794 19950511; AT 1995-992
     19950612; AT 1996-698 19960417; AT 1996-733 19960423.
GΙ
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
     Compds. of formula I (R1 = H or ester moiety, R2 = OY, NR4R5, N:R6, Y =
AB
Η,
     alkyl, alkenyl, acyl, carbamoyl, aryl, R4 = H, alkyl, alkenyl,
cycloalkyl,
     aryl, acyl, heterocyclyl, R5 = H, alkyl, alkenyl, cycloalkyl, aryl,
     heterocyclyl, C(SR7):NR8, C(NR9R10):Z, CR11:Z, R7 = alkyl or aryl, R8 =
Η,
     cycloalkyl, alkyl, R9 = H or alkyl, R10 = H, alkyl, OH, NH2, Ph, alkenyl,
     cycloalkyl, aryl, heterocyclyl, N:CHPhe, Phe = aryl, R9 and R10 together
     with nitrogen form a heterocyclyl, Z = O, S, NR13, R13 = H, alkyl or
     cycloalkyl, R11 = H, alkyl, aryl, cycloalkyl, or heterocyclyl, R4 and R5
     together with nitrogen form a heterocyclyl, R6 = heterocyclyl, Ac = Ac1,
     COCZ1:CZ2Z3, COCZ1:BDZ4, B = N, CH, Z1 = aryl, cycloalkyl, 1,4-hexadienyl
     or heterocyclyl, Z2 = H, alkyl, CH2CO2Z5, Z5 = H, alkyl, cycloalkyl, Z3 =
     H, alkyl, Z4 = H or org. radical, D = O or CH2), were prepd. thereof for
     use as pharmaceuticals, i.e. as antibacterial agents. Thus, II was
prepd.
     via condensation of formylcephemcarboxylic acid deriv. III in 4% aq. MeCN
     with guanidine IV in 1-2 N HCl. II has an MHK of 0.01 .mu.g/mL vs.
     Streptococcus pneumoniae (strain ATCC 49619) compared to 0.02 .mu.g/mL
for
     ceftriaxone.
     ANSWER 78 OF 148 REGISTRY COPYRIGHT 2000 ACS
L3
RN
     62869-99-2 REGISTRY
CN
     5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
     7-[(aminophenylacetyl)amino]-3-[[[(dihydro-2H-1,3-oxazin-3(4H)-
     yl)iminomethyl]hydrazono]methyl]-8-oxo-, [6R-(6.alpha.,7.beta.)]-,
     mono(trifluoroacetate) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
     2H-1,3-Oxazine, 5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid
CN
     deriv.
CN
     Acetic acid, trifluoro-, compd. with [6R-(6.alpha.,7.beta.)]-7-
     [(aminophenylacetyl)amino]-3-[[[(dihydro-2H-1,3-oxazin-3(4H)-
yl)iminomethyl]hydrazono]methyl]-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-
```

GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION:

CM 1

STEREOSEARCH

STN Files:

FS

MF

CRN 62733-46-4 CMF C21 H25 N7 O5 S

2-carboxylic acid (1:1)

C21 H25 N7 O5 S . C2 H F3 O2

CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

Absolute stereochemistry.
Double bond geometry unknown.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English).

CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GΙ

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2 = alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e.

morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; Prepared by M. Hale 308-4258 Page 181

R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me)

were prepd. by treating 3-formylcephem-4-carboxylates with III.

ANSWER 79 OF 148 REGISTRY COPYRIGHT 2000 ACS L3

RN 62777-35-9 REGISTRY

5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, CN

3-[[(2,6-dimethyl-4-morpholinyl)iminomethyl]hydrazono]methyl]-8-oxo-7-[(2thienylacetyl)amino]-, (6R,7R)- (9CI) (CA INDEX NAME) OTHER CA INDEX NAMES:

5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

3-[[(2,6-dimethyl-4-morpholinyl)iminomethyl]hydrazono]methyl]-8-oxo-7-[(2thienylacetyl)amino]-, [6R-(6.alpha.,7.beta.)]-

STEREOSEARCH

MF C21 H26 N6 O5 S2

CI COM

BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL LC (*File contains numerically searchable property data)

Absolute stereochemistry. Double bond geometry unknown.

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English).

CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GI

$$R^{3}NH$$
 (0) n $R^{3}NH$ (0) n $NHC=NR$ $CO_{2}R^{4}$ $NR^{1}R^{2}$ I O II

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2

alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me) were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 80 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62777-34-8 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

3-[[((2,5-dimethyl-4-morpholinyl)iminomethyl]hydrazono]methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, (6R,7R)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

3-[[(2,5-dimethyl-4-morpholinyl)iminomethyl]hydrazono]methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, [6R-(6.alpha.,7.beta.)]-

FS STEREOSEARCH

MF C21 H26 N6.05 S2

CI COM

LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL (*File contains numerically searchable property data)

Absolute stereochemistry.

Double bond geometry unknown.

1 REFERENCES IN FILE CA (1967 TO DATE) Prepared by M. Hale 308-4258

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru;
Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji
(Shionogi
and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English).
CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.
GI

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2 = alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me) were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 81 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62777-33-7 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[[[imino(3-methyl-4-morpholinyl)methyl]hydrazono]methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, (6R,7R)- (9CI) (CA INDEX NAME) OTHER CA INDEX NAMES:

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
3-[[imino(3-methyl-4-morpholinyl)methyl]hydrazono]methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, [6R-(6.alpha.,7.beta.)]-

FS STEREOSEARCH

MF C20 H24 N6 O5 S2

CI COM

LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL (*File contains numerically searchable property data)

Absolute stereochemistry. Double bond geometry unknown.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English). CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GΙ

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2 = alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH, Me)

were prepd. by treating 3-formylcephem-4-carboxylates with III.

- L3 ANSWER 82 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 62777-32-6 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[[imino(2-methyl-4-morpholinyl)methyl]hydrazono]methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, hydrobromide (2:1), [6R-(6.alpha.,7.beta.)]- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C20 H24 N6 O5 S2 . 1/2 Br H
- LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

CRN (56204-00-3)

Absolute stereochemistry. Prepared by M. Hale 308-4258

Double bond geometry unknown.

1/2 HBr

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English). CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GI

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2

alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me)

were prepd. by treating 3-formylcephem-4-carboxylates with III.

- L3 ANSWER 83 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 62766-40-9 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

7-amino-3-[[(imino-4-morpholinylmethyl)hydrazono]methyl]-8-oxo-, (6R, 7R)-,

bis(trifluoroacetate) (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

Prepared by M. Hale 308-4258

Page 186

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-amino-3-[[(imino-4-morpholinylmethyl)hydrazono]methyl]-8-oxo-, (6R-trans)-, bis(trifluoroacetate)

CN Acetic acid, trifluoro-, compd. with (6R-trans)-7-amino-3-[[(imino-4-

morpholinylmethyl)hydrazono]methyl]-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2ene-2-carboxylic acid (2:1)

FS STEREOSEARCH

MF C13 H18 N6 O4 S . 2 C2 H F3 O2

LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

CM 1

CRN 62766-39-6 CMF C13 H18 N6 O4 S

Absolute stereochemistry.
Double bond geometry unknown.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English). CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GI

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2 = alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C;

H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me) were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 84 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62766-39-6 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-amino-3-[[(imino-4-morpholinylmethyl)hydrazono]methyl]-8-oxo-, (6R,7R)-(9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-amino-3-[[(imino-4-morpholinylmethyl)hydrazono]methyl]-8-oxo-, (6R-trans)-

FS STEREOSEARCH

MF C13 H18 N6 O4 S

CI COM

LC STN Files: BEILSTEIN*

(*File contains numerically searchable property data)

Absolute stereochemistry.
Double bond geometry unknown.

- L3 ANSWER 85 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 62733-47-5 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 3-[[(dihydro-2H-1,3-oxazin-3(4H)-yl)iminomethyl]hydrazono]methyl]-7Prepared by M. Hale 308-4258
 Page 188

[[[[(1,1-dimethylethoxy)carbonyl]amino]phenylacetyl]amino]-8-oxo-,
[6R-(6.alpha.,7.beta.)]- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2H-1,3-Oxazine, 5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid deriv.

FS STEREOSEARCH

MF C26 H33 N7 O7 S

LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL (*File contains numerically searchable property data)

Absolute stereochemistry.

Double bond geometry unknown.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English).

CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GI

Me)

$$R^{3}NH$$
 $(O) n$
 $CH = NNHC = NR$
 $CO_{2}R^{4}$
 $NR^{1}R^{2}$
 I

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2 =

alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-02NC6H4CH2, Ph2CH,

were prepd. by treating 3-formylcephem-4-carboxylates with III. Prepared by M. Hale 308-4258 Page 189

L3 ANSWER 86 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62733-46-4 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-[(aminophenylacetyl)amino]-3-[[[(dihydro-2H-1,3-oxazin-3(4H)-yl)iminomethyl]hydrazono]methyl]-8-oxo-, [6R-(6.alpha.,7.beta.)]- (9CI)
(CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2H-1,3-Oxazine, 5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid deriv.

FS STEREOSEARCH

MF C21 H25 N7 O5 S

CI COM

LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL (*File contains numerically searchable property data)

Absolute stereochemistry.

Double bond geometry unknown.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English).

CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GI

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2 = alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. Prepared by M. Hale 308-4258

morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me)

were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 87 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62733-45-3 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)-3-[[[(dihydro-2H-1,3-oxazin-3(4H)-yl)iminomethyl]hydrazono]methyl]-8-oxo-, methyl ester, 5-oxide, [6R-(6.alpha.,7.beta.)]- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2H-1,3-Oxazine, 5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid deriv.

FS STEREOSEARCH

MF C22 H22 N6 O7 S

LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

Absolute stereochemistry.

Double bond geometry unknown.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English). CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GΙ

$$R^{3}NH$$
 $(O)_{n}$ $CH = NNHC = NR$ $CO_{2}R^{4}$ $NR^{1}R^{2}$ I $R^{3}NH$ $(O)_{n}$ N OH OH OH OH

Prepared by M. Hale 308-4258

Page 191

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2

alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me)

were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 88 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62733-44-2 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

3-[[[(dihydro-2H-1,3-oxazin-3(4H)-yl)iminomethyl]hydrazono]methyl]-8-oxo-7[(2-thienylacetyl)amino]-, diphenylmethyl ester, (6R-trans)- (9CI) (CA
INDEX NAME)

OTHER CA INDEX NAMES:

CN 2H-1,3-Oxazine, 5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid deriv.

FS STEREOSEARCH

MF C32 H32 N6 O5 S2

LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL (*File contains numerically searchable property data)

Absolute stereochemistry.
Double bond geometry unknown.

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English). CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GI

R3NH (O) n CH = NNHC = NR
$$CO_2R^4$$
 NR1R2

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2

alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me) were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 89 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62733-43-1 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

3-[[(dihydro-2H-1,3-oxazin-3(4H)-yl)iminomethyl]hydrazono]methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, monosodium salt, (6R-trans)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2H-1,3-Oxazine, 5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid deriv.

FS STEREOSEARCH

MF C19 H22 N6 O5 S2 . Na

LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

CRN (62733-24-8)

Absolute stereochemistry.

Double bond geometry unknown.

Na

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English). CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GΙ

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2

alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me)

were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 90 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62733-42-0 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

7-amino-3-[[[(dihydro-2H-1,3-oxazin-3(4H)-yl)iminomethyl]hydrazono]methyl]-8-oxo-, (6R-trans)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME) OTHER CA INDEX NAMES:

CN 2H-1,3-Oxazine, 5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid deriv.

CN Acetic acid, trifluoro-, compd. with (6R-trans)-7-amino-3-[[[(dihydro-2H-1,3-oxazin-3(4H)-yl)iminomethyl]hydrazono]methyl]-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid (2:1)

FS STEREOSEARCH

MF C13 H18 N6 O4 S . 2 C2 H F3 O2

LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

CM 1

CRN 62733-38-4 CMF C13 H18 N6 O4 S

Absolute stereochemistry.
Double bond geometry unknown.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English). CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GI

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2

alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me)

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Page 195

were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 91 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62733-41-9 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

7-amino-3-[[[(dihydro-2H-1,3-oxazin-3(4H)-yl)iminomethyl]hydrazono]methyl]-8-oxo-, (4-nitrophenyl)methyl ester, (6R-trans)- (9CI) (CA INDEX NAME) OTHER CA INDEX NAMES:

CN 2H-1,3-Oxazine, 5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid deriv.

FS STEREOSEARCH

MF C20 H23 N7 O6 S

LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL (*File contains numerically searchable property data)

Absolute stereochemistry.
Double bond geometry unknown.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English).

CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GΙ

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2 Prepared by M. Hale 308-4258 Page 196 alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me)

were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 92 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62733-40-8 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

3-[[[(dihydro-2H-1,3-oxazin-3(4H)-yl)iminomethyl]hydrazono]methyl]-8-oxo-7[(phenoxyacetyl)amino]-, (6R-trans)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:

CN 2H-1,3-Oxazine, 5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid deriv.

FS STEREOSEARCH

MF C21 H24 N6 O6 S

LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

Absolute stereochemistry.

Double bond geometry unknown.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English).

CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GΙ

$$R^{3}NH$$
 (0) n $R^{3}NH$ (0) n N OH OH OH $CH = NNHC = NR$ $CO_{2}R^{4}$ $NR^{1}R^{2}$ I O II

Prepared by M. Hale 308-4258

Page 197

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2

alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me)

were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 93 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62733-39-5 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)-3-[[[(dihydro-2H-1,3-oxazin-3(4H)-yl)iminomethyl]hydrazono]methyl]-8-oxo-, (6R-trans)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2H-1,3-Oxazine, 5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid deriv.

FS STEREOSEARCH

MF C21 H20 N6 O6 S

LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

Absolute stereochemistry.

Double bond geometry unknown.

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English). CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GΙ

$$R^{3}NH$$
 $(O)_{n}$ $R^{3}NH$ $(O)_{n}$ OH OH $CH = NNHC = NR$ $CO_{2}R^{4}$ $NR^{1}R^{2}$ I

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2

alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me) were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 94 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62733-38-4 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

7-amino-3-[([(dihydro-2H-1,3-oxazin-3(4H)-yl)iminomethyl]hydrazono]methyl]-8-oxo-, (6R-trans)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2H-1,3-Oxazine, 5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid deriv.

FS STEREOSEARCH

MF C13 H18 N6 O4 S

CI COM

LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

Absolute stereochemistry. Double bond geometry unknown.

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

Prepared by M. Hale 308-4258

Page 199

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English). CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GI

The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2 AB alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me) were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 95 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62733-36-2 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[1-[(imino-4-morpholinylmethyl)hydrazono]ethyl]-8-oxo-7-[(2thienylacetyl)amino]-, (6R-trans)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF. C20 H24 N6 O5 S2

STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL LC

Absolute stereochemistry. Double bond geometry unknown.

1 REFERENCES IN FILE CA (1967 TO DATE) 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

(English). Page 200 and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. Prepared by M. Hale 308-4258

$$R^{3}NH$$
 (0) n $R^{3}NH$ (0) n N OH OH OH $CH = NNHC = NR$ $NR^{1}R^{2}$ I

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2 = alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me) were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 96 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62733-35-1 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[[(imino-4-morpholinylmethyl)hydrazono]methyl]-7-methoxy-7-[[(2-nitrophenyl)thio]amino]-8-oxo-, (6R-cis)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C20 H23 N7 O7 S2

LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

Absolute stereochemistry. Double bond geometry unknown.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru;
Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji
(Shionogi Prepared by M. Hale 308-4258 Page 201

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English). CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GI

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2 = alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me) were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 97 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62733-34-0 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[[(imino-4-morpholinylmethyl)hydrazono]methyl]-8-oxo-7-[[(2,2,2-trichloroethoxy)carbonyl]amino]-, (6R-trans)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C16 H19 C13 N6 O6 S

CI COM

LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL . (*File contains numerically searchable property data)

Absolute stereochemistry.

Double bond geometry unknown.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru;
Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji
Prepared by M. Hale 308-4258
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and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English). CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GI

$$R^{3}NH$$
 $(0)_{n}$ $R^{3}NH$ $(0)_{n}$ N OH OH OH $CH=NNHC=NR$ $NR^{1}R^{2}$ I O OH

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2 = alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me) were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 98 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62733-33-9 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[(1,1-dimethylethoxy)carbonyl]amino]-3-[[(imino-4-morpholinylmethyl)hydrazono]methyl]-8-oxo-, (6R-trans)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C18 H26 N6 O6 S

CI COM

LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL (*File contains numerically searchable property data)

Absolute stereochemistry.

Double bond geometry unknown.

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Prepared by M. Hale 308-4258 Page 203 Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English).

CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GI

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2 =

alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me)

were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 99 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62733-32-8 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[(imino-4-morpholinylmethyl)hydrazono]methyl]-8-oxo-7-[(3-thienylacetyl)amino]-, (6R-trans)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C19 H22 N6 O5 S2

CI COM

LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL (*File contains numerically searchable property data)

Absolute stereochemistry. Double bond geometry unknown.

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

Prepared by M. Hale 308-4258

Page 204

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English). CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GI

$$R^{3}NH$$
 (0) n
 $CH = NNHC = NR$
 $CO_{2}R^{4}$
 $NR^{1}R^{2}$
 I
 $R^{3}NH$
 (0) n
 $R^{3}NH$
 (0) n

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2 = alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me) were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 100 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62733-31-7 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
3-[[(imino-4-morpholinylmethyl)hydrazono]methyl]-8-oxo-7[(phenylacetyl)amino]-, hydrobromide (2:1), (6R-trans)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C21 H24 N6 O5 S . 1/2 Br H

LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

Absolute stereochemistry.

Double bond geometry unknown.

1/2 HBr

Prepared by M. Hale 308-4258

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English) CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GI

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2

alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me) were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 101 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62733-30-6 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

(CA INDEX NAME)

FS STEREOSEARCH

MF C26 H33 N7 O7 S

CI COM

LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL (*File contains numerically searchable property data)

Absolute stereochemistry.
Double bond geometry unknown.

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English). CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GI

$$R^{3}NH$$
 $CH = NNHC = NR$
 $CO_{2}R^{4}$
 $NR^{1}R^{2}$
 $R^{3}NH$
 $R^{3}NH$

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2

alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me)

were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 102 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62733-29-3 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

7-[(aminophenylacetyl)amino]-3-[[(imino-4-morpholinylmethyl)hydrazono]meth yl]-8-oxo-, [6R-(6.alpha.,7.beta.)]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C21 H25 N7 O5 S

CI COM

LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL (*File contains numerically searchable property data)
Prepared by M. Hale 308-4258

Page 207

Absolute stereochemistry.

Double bond geometry unknown.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English) CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

 $R^{3}NH$ $(O)_{n}$ $R^{3}NH$ $(O)_{n}$ $R^{3}NH$ $(O)_{n}$ $R^{3}NH$ $(O)_{n}$ N $(O)_{n}$ N $(O)_{n}$ $(O)_{n$

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2

alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

ОН

II

Me) were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 103 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62733-28-2 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

7-[[[(2,3-dihydro-1-methyl-1H-tetrazol-5-yl)thio]acetyl]amino]-3-[[(imino-4-morpholinylmethyl)hydrazono]methyl]-8-oxo-, (6R-trans)- (9CI) (CA INDEX

NAME)

GI

Prepared by M. Hale 308-4258

FS STEREOSEARCH

MF C17 H24 N10 O5 S2

LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

Absolute stereochemistry.

Double bond geometry unknown.

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English)

CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GI

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2

alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me) were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 104 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62733-27-1 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[[(imino-4-morpholinylmethyl)hydrazono]methyl]-8-oxo-7-Prepared by M. Hale 308-4258

Page 209

[(phenoxyacetyl)amino]-, (6R-trans)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C21 H24 N6 O6 S

CI COM

LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL (*File contains numerically searchable property data)

Absolute stereochemistry.

Double bond geometry unknown.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English).

CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GΙ

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2 =

alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me) were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 105 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62733-26-0 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, Prepared by M. Hale 308-4258

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3-[[(imino-4-thiomorpholinylmethyl)hydrazono]methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, (6R-trans)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Thiomorpholine, 5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid deriv.

FS STEREOSEARCH

MF C19 H22 N6 O4 S3

CI COM

LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL (*File contains numerically searchable property data)

Absolute stereochemistry.

Double bond geometry unknown.

1 REFERENCES IN FILE CA (1967 TO DATE) 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English).

CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GI

Me)

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2 = alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

were prepd. by treating 3-formylcephem-4-carboxylates with III. Prepared by M. Hale 308-4258 Page 211

L3 ANSWER 106 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62733-25-9 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[[(imino-3-thiazolidinylmethyl)hydrazono]methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, (6R-trans)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C18 H20 N6 O4 S3

CI COM

LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL (*File contains numerically searchable property data)

Absolute stereochemistry.

Double bond geometry unknown.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English).

CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GΙ

Me)

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2 = alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

were prepd. by treating 3-formylcephem-4-carboxylates with III.
Prepared by M. Hale 308-4258

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L3 ANSWER 107 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62733-24-8 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

3-[[[(dihydro-2H-1,3-oxazin-3(4H)-yl)iminomethyl]hydrazono]methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, (6R-trans)- (9CI) (CA INDEX NAME) OTHER CA INDEX NAMES:

CN 2H-1,3-Oxazine, 5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid deriv.

FS STEREOSEARCH

MF C19 H22 N6 O5 S2

CI COM

LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL (*File contains numerically searchable property data)

Absolute stereochemistry. Double bond geometry unknown.

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English).

CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GI

$$R^{3}NH$$
 $(O)_{n}$ $CH = NNHC = NR$ $CO_{2}R^{4}$ $NR^{1}R^{2}$ I O $R^{3}NH$ $(O)_{n}$ OH OH OH OH

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2

alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, Prepared by M. Hale 308-4258 Page 213

H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-02NC6H4CH2, Ph2CH,

Me)

were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 108 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62733-23-7 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

3-[[[imino(tetrahydro-2H-1,2-oxazin-2-yl)methyl]hydrazono]methyl]-8-oxo-7[(2-thienylacetyl)amino]-, (6R-trans)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:

CN 2H-1,2-Oxazine, 5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid deriv.

FS STEREOSEARCH

MF C19 H22 N6 O5 S2

CI COM

LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL (*File contains numerically searchable property data)

Absolute stereochemistry.

Double bond geometry unknown.

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English).

CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GΙ

Prepared by M. Hale 308-4258

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2

alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me) were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 109 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62733-22-6 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[[(ethylamino)-4-morpholinylmethylene]hydrazono]methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, hydriodide (2:1), (6R-trans)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C21 H26 N6 O5 S2 . 1/2 H I

LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

Absolute stereochemistry.

Double bond geometry unknown.

● 1/2 HI

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English). CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GΙ

$$R^{3}NH$$
 $(O)_{n}$ $R^{3}NH$ $(O)_{n}$ OH $(O)_{n}$ OH $(O)_{n}$ $(O)_$

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2 = alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C;

H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, C13CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me) were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 110 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62733-21-5 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[[(imino-4-morpholinylmethyl)hydrazono]methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, hydriodide (2:1), (6R-trans)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C19 H22 N6 O5 S2 . 1/2 H I

LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

CRN (62733-20-4)

Absolute stereochemistry.

Double bond geometry unknown.

• 1/2 HI

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi Prepared by M. Hale 308-4258 Page 216 and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English). CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GI

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2 = alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me) were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 111 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62733-20-4 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[[(imino-4-morpholinylmethyl)hydrazono]methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, (6R-trans)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C19 H22 N6 O5 S2

ČI COM

LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL (*File contains numerically searchable property data)

Absolute stereochemistry.
Double bond geometry unknown.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru;
Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji
Prepared by M. Hale 308-4258
Page 217

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English). CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GI

$$R^{3}NH$$
 (O) n $R^{3}NH$ (O) n OH $CH = NNHC = NR$ $NR^{1}R^{2}$ I

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2 = alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me) were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 112 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62733-19-1 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[[(imino-4-morpholinylmethyl)hydrazono]methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, hydrobromide (2:1), (6R-trans)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C19 H22 N6 O5 S2 . 1/2 Br H

LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

CRN (62733-20-4)

Absolute stereochemistry. Double bond geometry unknown.

● 1/2 HBr

1 REFERENCES IN FILE CA (1967 TO DATE) Prepared by M. Hale 308-4258

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English).

CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GI

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2

alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me)

were prepd. by treating 3-formylcephem-4-carboxylates with III.

- L3 ANSWER 113 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 62733-18-0 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
- 3-[[(2,5-dihydro-1H-pyrrol-1-yl)iminomethyl]hydrazono]methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, (6R-trans)- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C19 H20 N6 O4 S2
- CI COM
- LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL (*File contains numerically searchable property data)

Absolute stereochemistry. Double bond geometry unknown.

Prepared by M. Hale 308-4258

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English).

CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GΙ

The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2 AΒ

alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me)

were prepd. by treating 3-formylcephem-4-carboxylates with III.

ANSWER 114 OF 148 REGISTRY COPYRIGHT 2000 ACS L3

62733-17-9 REGISTRY RN

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[[(imino-1-piperidinylmethyl)hydrazono]methyl]-8-oxo-7-[(2thienylacetyl)amino]-, (6R-trans)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C20 H24 N6 O4 S2

CI COM

LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL (*File contains numerically searchable property data)

Absolute stereochemistry. Double bond geometry unknown.

Prepared by M. Hale 308-4258

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English).

CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GΙ

$$R^{3}NH$$
 $(O) n$
 $CH = NNHC = NR$
 $CO_{2}R^{4}$
 $NR^{1}R^{2}$
 I
 $R^{3}NH$
 $(O) n$
 $(O) n$

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2 = alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C;

H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, C13CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me) were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 115 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62733-16-8 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[[(imino-1-pyrrolidinylmethyl)hydrazono]methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, (6R-trans)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C19 H22 N6 O4 S2

CI COM

LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL (*File contains numerically searchable property data)

Absolute stereochemistry. Double bond geometry unknown.

Prepared by M. Hale 308-4258

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English). CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GΙ

$$R^{3}NH$$
 $(O)_{n}$
 $CH=NNHC=NR$
 $CO_{2}R^{4}$
 $NR^{1}R^{2}$
 I
 $R^{3}NH$
 $(O)_{n}$
 $R^{3}NH$
 $(O)_{n}$
 $R^{3}NH$
 $(O)_{n}$
 $R^{3}NH$
 $(O)_{n}$
 $R^{3}NH$
 $(O)_{n}$
 N
 $(O)_{n}$
 $(O)_{n}$

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2

alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me)

were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 116 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62732-98-3 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
7-(acetylamino)-3-[[[(dihydro-2H-1,3-oxazin-3(4H)yl)iminomethyl]hydrazono]methyl]-8-oxo-, (4-nitrophenyl)methyl ester,
(6R-trans)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2H-1,3-Oxazine, 5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid deriv.

FS STEREOSEARCH

MF C22 H25 N7 O7 S

LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL (*File contains numerically searchable property data)

Absolute stereochemistry.
Double bond geometry unknown.

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English).

CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GΙ

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2 = ...

alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH, Me)

were prepd. by treating 3-formylcephem-4-carboxylates with III.

- L3 ANSWER 117 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 62732-96-1 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)-3-[[[(dihydro-2H-1,3-oxazin-3(4H)-yl)iminomethyl]hydrazono]methyl]-8-oxo-, methyl ester, (6R-trans)-(9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2H-1,3-Oxazine, 5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid deriv. Prepared by M. Hale 308-4258 Page 223

FS STEREOSEARCH

MF C22 H22 N6 O6 S

LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL (*File contains numerically searchable property data)

Absolute stereochemistry.
Double bond geometry unknown.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English).

CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GI

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2

alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me) were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 118 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62732-95-0 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, Prepared by M. Hale 308-4258

Page 224

3-[[[(dihydro-2H-1,3-oxazin-3(4H)-yl)iminomethyl]hydrazono]methyl]-8-oxo-7[(2-thienylacetyl)amino]-, diphenylmethyl ester, 5-oxide,
[6R-(6.alpha.,7.beta.)]- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2H-1,3-Oxazine, 5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid deriv.

FS STEREOSEARCH

MF C32 H32 N6 O6 S2

LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL (*File contains numerically searchable property data)

Absolute stereochemistry.

Double bond geometry unknown.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English).

CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GI

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2 = alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH, Prepared by M. Hale 308-4258

were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 119 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 62732-94-9 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[[(dihydro-2H-1,3-oxazin-3(4H)-yl)iminomethyl]hydrazono]methyl]-7-[[(1,1-dimethylethoxy)carbonyl]amino]-8-oxo-, (4-nitrophenyl)methyl ester,

(6R-trans)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2H-1,3-Oxazine, 5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid deriv.

FS STEREOSEARCH

MF C25 H31 N7 O8 S

LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL (*File contains numerically searchable property data)

Absolute stereochemistry. Double bond geometry unknown.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English). CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GI

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2 = alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me) were prepd. by treating 3-formylcephem-4-carboxylates with III.

L3 ANSWER 120 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 56376-57-9 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-amino-3-[[(imino-4-morpholinylmethyl)hydrazono]methyl]-8-oxo-, monohydrobromide, (6R,7R)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-amino-3-[[(imino-4-morpholinylmethyl)hydrazono]methyl]-8-oxo-, monohydrobromide, (6R-trans)-

FS STEREOSEARCH

MF C13 H18 N6 O4 S . Br H

LC STN Files: CA, CAPLUS

CRN (62766-39-6)

Absolute stereochemistry.
Double bond geometry unknown.

• HBr

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 83:58855 Pharmaceutical cephalosporins. Yoshioka, Mitsuru; Sendo, Yuji; Murakami, Masayuki; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). Ger. Offen. DE 2450618 19750430, 56 pp. (German).

CODEN: GWXXBX. PRIORITY: JP 1973-120328 19731025.

GI For diagram(s), see printed CA Issue.

AB Approx. 60 bactericides (no data) I (e.g., R1 = 2-thienyl, PhCH(NH2), PhCH2, 2-furyl; R2, R3 = H, Et, allyl, Ph; NR2R3 = morpholino) were prepd.

in 41-100% yield by treatment of II with H2NNHC(:NH)NR2R3. P-nitrophenyl Prepared by M. Hale 308-4258 Page 227 3-formyl-7-tert-butoxycarbonylamino-3-cephem-4-carboxylate reacted with 4,4-(3-oxopentamethylene) quanylhydrazine-HBr and THF for 16.5 hr at room temp. to give 72% of the

3-[[4,4-(3-oxopentamethylene)quanylhydrazono]meth yl] cephem deriv.

ANSWER 121 OF 148 REGISTRY COPYRIGHT 2000 ACS L3

RN 56210-08-3 REGISTRY

5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, CN 3-[((imino-1-piperidinylmethyl)hydrazono]methyl]-8-oxo-7-[(2thienylacetyl)amino]-, monohydriodide, (6R-trans)- (9CI) (CA INDEX NAME) FS · STEREOSEARCH

C20 H24 N6 O4 S2 . H I MF

LC STN Files: CA, CAPLUS

CRN (62733-17-9)

Absolute stereochemistry. Double bond geometry unknown.

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 83:58855 Pharmaceutical cephalosporins. Yoshioka, Mitsuru; Sendo, Yuji; Murakami, Masayuki; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). Ger. Offen. DE 2450618 19750430, 56 pp. (German).

CODEN: GWXXBX. PRIORITY: JP 1973-120328 19731025.

GI For diagram(s), see printed CA Issue.

AΒ Approx. 60 bactericides (no data) I (e.g., R1 = 2-thienyl, PhCH(NH2), PhCH2, 2-furyl; R2, R3 = H, Et, allyl, Ph; NR2R3 = morpholino) were prepd.

in 41-100% yield by treatment of II with H2NNHC(:NH)NR2R3. P-nitrophenyl 3-formyl-7-tert-butoxycarbonylamino-3-cephem-4-carboxylate reacted with 4,4-(3-oxopentamethylene) guanylhydrazine-HBr and THF for 16.5 hr at room temp. to give 72% of the

3-[[4,4-(3-oxopentamethylene)guanylhydrazono]meth yl] cephem deriv.

ANSWER 122 OF 148 REGISTRY COPYRIGHT 2000 ACS 1.3

RN

56204-21-8 REGISTRY Prepared by M. Hale 308-4258

Page 228

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
3-[[(imino-4-morpholinylmethyl)hydrazono]methyl]-7-methoxy-8-oxo-7-[(2-thienylacetyl)amino]-, monohydrobromide, (6R-cis)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C20 H24 N6 O6 S2 . Br H

Absolute stereochemistry.

Double bond geometry unknown.

STN Files:

LC

CA, CAPLUS

• HBr

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 83:58855 Pharmaceutical cephalosporins. Yoshioka, Mitsuru; Sendo, Yuji; Murakami, Masayuki; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). Ger. Offen. DE 2450618 19750430, 56 pp. (German).

CODEN: GWXXBX. PRIORITY: JP 1973-120328 19731025.

GI For diagram(s), see printed CA Issue.

AB Approx. 60 bactericides (no data) I (e.g., R1 = 2-thienyl, PhCH(NH2), PhCH2, 2-furyl; R2, R3 = H, Et, allyl, Ph; NR2R3 = morpholino) were prepd.

in 41-100% yield by treatment of II with H2NNHC(:NH)NR2R3. P-nitrophenyl 3-formyl-7-tert-butoxycarbonylamino-3-cephem-4-carboxylate reacted with 4,4-(3-oxopentamethylene)guanylhydrazine-HBr and THF for 16.5 hr at room temp. to give 72% of the

3-[[4,4-(3-oxopentamethylene)guanylhydrazono]meth yl] cephem deriv.

- L3 ANSWER 123 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 56204-20-7 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 3-[[(imino-4-morpholinylmethyl)hydrazono]methyl]-7-[[(2nitrophenyl)thio]amino]-8-oxo-, monohydrobromide, (6R-trans)- (9CI) (CA
 INDEX NAME)
- FS STEREOSEARCH
- MF C19 H21 N7 O6 S2 . Br H
- LC STN Files: CA, CAPLUS
 Prepared by M. Hale 308-4258

Page 229

Absolute stereochemistry.

Double bond geometry unknown.

HBr

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 83:58855 Pharmaceutical cephalosporins. Yoshioka, Mitsuru; Sendo, Yuji; Murakami, Masayuki; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). Ger. Offen. DE 2450618 19750430, 56 pp. (German).

CODEN: GWXXBX. PRIORITY: JP 1973-120328 19731025.

GI For diagram(s), see printed CA Issue.

AB Approx. 60 bactericides (no data) I (e.g., R1 = 2-thienyl, PhCH(NH2), PhCH2, 2-furyl; R2, R3 = H, Et, allyl, Ph; NR2R3 = morpholino) were prepd.

in 41-100% yield by treatment of II with H2NNHC(:NH)NR2R3. P-nitrophenyl 3-formyl-7-tert-butoxycarbonylamino-3-cephem-4-carboxylate reacted with 4,4-(3-oxopentamethylene)guanylhydrazine-HBr and THF for 16.5 hr at room temp. to give 72% of the

3-[[4,4-(3-oxopentamethylene)guanylhydrazono]meth yl] cephem deriv.

L3 ANSWER 124 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 56204-19-4 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[[(imino-4-morpholinylmethyl)hydrazono]methyl]-8-oxo-7-[[(2,2,2-trichloroethoxy)carbonyl]amino]-, monohydrobromide, (6R-trans)- (9CI)

(CA

INDEX NAME)

FS STEREOSEARCH

MF C16 H19 C13 N6 O6 S . Br H

LC STN Files: CA, CAPLUS

CRN (62733-34-0)

Absolute stereochemistry.
Double bond geometry unknown.

C13C O
$$\frac{H}{N}$$
 $\frac{H}{N}$ $\frac{H}{N}$ $\frac{NH}{N}$ \frac{NH}

• HBr

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 83:58855 Pharmaceutical cephalosporins. Yoshioka, Mitsuru; Sendo, Yuji; Murakami, Masayuki; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). Ger. Offen. DE 2450618 19750430, 56 pp. (German).

CODEN: GWXXBX. PRIORITY: JP 1973-120328 19731025.

GI For diagram(s), see printed CA Issue.

AB Approx. 60 bactericides (no data) I (e.g., R1 = 2-thienyl, PhCH(NH2), PhCH2, 2-furyl; R2, R3 = H, Et, allyl, Ph; NR2R3 = morpholino) were prepd.

in 41-100% yield by treatment of II with H2NNHC(:NH)NR2R3. P-nitrophenyl 3-formyl-7-tert-butoxycarbonylamino-3-cephem-4-carboxylate reacted with 4,4-(3-oxopentamethylene)guanylhydrazine-HBr and THF for 16.5 hr at room temp. to give 72% of the

3-[[4,4-(3-oxopentamethylene)guanylhydrazono]meth yl] cephem deriv.

- L3 ANSWER 125 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 56204-18-3 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 7-[[(1,1-dimethylethoxy)carbonyl]amino]-3-[[(imino-4morpholinylmethyl)hydrazono]methyl]-8-oxo-, monohydrobromide, (6R-trans)(9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C18 H26 N6 O6 S . Br H
- LC STN Files: CA, CAPLUS
- CRN (62733-33-9)

Absolute stereochemistry. Double bond geometry unknown.

HBr

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 83:58855 Pharmaceutical cephalosporins. Yoshioka, Mitsuru; Sendo, Yuji; Murakami, Masayuki; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). Ger. Offen. DE 2450618 19750430, 56 pp. (German).

CODEN: GWXXBX. PRIORITY: JP 1973-120328 19731025.

GI For diagram(s), see printed CA Issue.

AB Approx. 60 bactericides (no data) I (e.g., R1 = 2-thienyl, PhCH(NH2), PhCH2, 2-furyl; R2, R3 = H, Et, allyl, Ph; NR2R3 = morpholino) were prepd.

in 41-100% yield by treatment of II with H2NNHC(:NH)NR2R3. P-nitrophenyl 3-formyl-7-tert-butoxycarbonylamino-3-cephem-4-carboxylate reacted with 4,4-(3-oxopentamethylene)guanylhydrazine-HBr and THF for 16.5 hr at room temp. to give 72% of the

3-[[4,4-(3-oxopentamethylene)guanylhydrazono]meth yl] cephem deriv.

L3 ANSWER 126 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 56204-17-2 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
3-[(imino-4-morpholinylmethyl)hydrazono]methyl]-8-oxo-7-[(1H-tetrazol-1-ylacetyl)amino]-, monohydrobromide, (6R-trans)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH
MF C16 H20 N10 O5 S . Br H

LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL (*File contains numerically searchable property data)

Absolute stereochemistry. Double bond geometry unknown.

HBr

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English).
CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.
GI

 $(Q)_n$

OH

ΙI

 $R^{3}NH$ (0) n CH = NNHC = NR $CO_{2}R^{4}$ $NR^{1}R^{2}$ I

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2 = alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C;

H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, C13CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

were prepd. by treating 3-formylcephem-4-carboxylates with III.

REFERENCE 2: 83:58855 Pharmaceutical cephalosporins. Yoshioka, Mitsuru; Sendo, Yuji; Murakami, Masayuki; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). Ger. Offen. DE 2450618 19750430, 56 pp. (German).

CODEN: GWXXBX. PRIORITY: JP 1973-120328 19731025.

GI For diagram(s), see printed CA Issue.

Me)

AB Approx. 60 bactericides (no data) I (e.g., R1 = 2-thienyl, PhCH(NH2), Prepared by M. Hale 308-4258 Page 233

PhCH2, 2-furyl; R2, R3 = H, Et, allyl, Ph; NR2R3 = morpholino) were prepd.

in 41-100% yield by treatment of II with H2NNHC(:NH)NR2R3. P-nitrophenyl 3-formyl-7-tert-butoxycarbonylamino-3-cephem-4-carboxylate reacted with 4,4-(3-oxopentamethylene)guanylhydrazine-HBr and THF for 16.5 hr at room temp. to give 72% of the

3-[[4,4-(3-oxopentamethylene)guanylhydrazono]meth yl] cephem deriv.

L3 ANSWER 127 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 56204-16-1 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[(imino-4-morpholinylmethyl)hydrazono]methyl]-8-oxo-7-[(3-thienylacetyl)amino]-, monohydrobromide, (6R-trans)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C19 H22 N6 O5 S2 . Br H

LC STN Files: CA, CAPLUS

CRN (62733-32-8)

Absolute stereochemistry.

Double bond geometry unknown.

• HBr

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 83:58855 Pharmaceutical cephalosporins. Yoshioka, Mitsuru; Sendo, Yuji; Murakami, Masayuki; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). Ger. Offen. DE 2450618 19750430, 56 pp. (German).

CODEN: GWXXBX. PRIORITY: JP 1973-120328 19731025.

GI For diagram(s), see printed CA Issue.

AB Approx. 60 bactericides (no data) I (e.g., R1 = 2-thienyl, PhCH(NH2), PhCH2, 2-furyl; R2, R3 = H, Et, allyl, Ph; NR2R3 = morpholino) were prepd.

in 41-100% yield by treatment of II with H2NNHC(:NH)NR2R3. P-nitrophenyl 3-formyl-7-tert-butoxycarbonylamino-3-cephem-4-carboxylate reacted with 4,4-(3-oxopentamethylene) guanylhydrazine-HBr and THF for 16.5 hr at room temp. to give 72% of the

3-[[4,4-(3-oxopentamethylene)guanylhydrazono]meth Prepared by M. Hale 308-4258

yl] cephem deriv.

L3 ANSWER 128 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 56204-15-0 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

7-[(2-furanylacetyl)amino]-3-[[(imino-4-morpholinylmethyl)hydrazono]methyl]-8-oxo-, monohydrobromide, (6R-trans)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C19 H22 N6 O6 S . Br H

LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL (*File contains numerically searchable property data)

Absolute stereochemistry.

Double bond geometry unknown.

• HBr

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English).

CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GI

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2 = alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. Prepared by M. Hale 308-4258

morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me)

were prepd. by treating 3-formylcephem-4-carboxylates with III.

REFERENCE 2: 83:58855 Pharmaceutical cephalosporins. Yoshioka, Mitsuru; Sendo, Yuji; Murakami, Masayuki; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). Ger. Offen. DE 2450618 19750430, 56 pp. (German).

CODEN: GWXXBX. PRIORITY: JP 1973-120328 19731025.

GI For diagram(s), see printed CA Issue.

AB Approx. 60 bactericides (no data) I (e.g., R1 = 2-thienyl, PhCH(NH2), PhCH2, 2-furyl; R2, R3 = H, Et, allyl, Ph; NR2R3 = morpholino) were prepd.

in 41-100% yield by treatment of II with H2NNHC(:NH)NR2R3. P-nitrophenyl 3-formyl-7-tert-butoxycarbonylamino-3-cephem-4-carboxylate reacted with 4,4-(3-oxopentamethylene)guanylhydrazine-HBr and THF for 16.5 hr at room temp. to give 72% of the

3-[[4,4-(3-oxopentamethylene)guanylhydrazono]meth yl] cephem deriv.

L3 ANSWER 129 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 56204-14-9 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
3-[(imino-4-morpholinylmethyl)hydrazono]methyl]-8-oxo-7[(phenylacetyl)amino]-, monohydrobromide, (6R-trans)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C21 H24 N6 O5 S . Br H

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry unknown.

• HBr

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 83:58855 Pharmaceutical cephalosporins. Yoshioka, Mitsuru; Prepared by M. Hale 308-4258 Page 236 Sendo, Yuji; Murakami, Masayuki; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). Ger. Offen. DE 2450618 19750430, 56 pp. (German).

CODEN: GWXXBX. PRIORITY: JP 1973-120328 19731025.

GI For diagram(s), see printed CA Issue.

AB Approx. 60 bactericides (no data) I (e.g., R1 = 2-thienyl, PhCH(NH2), PhCH2, 2-furyl; R2, R3 = H, Et, allyl, Ph; NR2R3 = morpholino) were prepd.

in 41-100% yield by treatment of II with H2NNHC(:NH)NR2R3. P-nitrophenyl 3-formyl-7-tert-butoxycarbonylamino-3-cephem-4-carboxylate reacted with 4,4-(3-oxopentamethylene)guanylhydrazine-HBr and THF for 16.5 hr at room temp. to give 72% of the

3-[[4,4-(3-oxopentamethylene)guanylhydrazono]meth yl] cephem deriv.

L3 ANSWER 130 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 56204-13-8 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

7-[[[[(1,1-dimethylethoxy)carbonyl]amino]phenylacetyl]amino]-3-[[(imino-4-morpholinylmethyl)hydrazono]methyl]-8-oxo-, monohydrobromide, [6R-(6.alpha.,7.beta.)]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C26 H33 N7 O7 S . Br H

LC STN Files: CA, CAPLUS

CRN (62733-30-6)

Absolute stereochemistry.

Double bond geometry unknown.

• HBr

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 83:58855 Pharmaceutical cephalosporins. Yoshioka, Mitsuru; Sendo, Yuji; Murakami, Masayuki; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). Ger. Offen. DE 2450618 19750430, 56 pp. (German).

CODEN: GWXXBX. PRIORITY: JP 1973-120328 19731025. Prepared by M. Hale 308-4258

GI For diagram(s), see printed CA Issue.

AB Approx. 60 bactericides (no data) I (e.g., R1 = 2-thienyl, PhCH(NH2), PhCH2, 2-furyl; R2, R3 = H, Et, allyl, Ph; NR2R3 = morpholino) were prepd.

in 41-100% yield by treatment of II with H2NNHC(:NH)NR2R3. P-nitrophenyl 3-formyl-7-tert-butoxycarbonylamino-3-cephem-4-carboxylate reacted with 4,4-(3-oxopentamethylene)guanylhydrazine-HBr and THF for 16.5 hr at room temp. to give 72% of the

3-[[4,4-(3-oxopentamethylene)guanylhydrazono]meth yl] cephem deriv.

L3 ANSWER 131 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 56204-12-7 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

7-[(aminophenylacetyl)amino]-3-[[(imino-4-morpholinylmethyl)hydrazono]meth yl]-8-oxo-, monohydrobromide, [6R-(6.alpha.,7.beta.)]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C21 H25 N7 O5 S . Br H

LC STN Files: CA, CAPLUS

CRN (62733-29-3) .

Absolute stereochemistry.

Double bond geometry unknown.

• HBr

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 83:58855 Pharmaceutical cephalosporins. Yoshioka, Mitsuru; Sendo, Yuji; Murakami, Masayuki; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). Ger. Offen. DE 2450618 19750430, 56 pp. (German).

CODEN: GWXXBX. PRIORITY: JP 1973-120328 19731025.

GI For diagram(s), see printed CA Issue.

AB Approx. 60 bactericides (no data) I (e.g., R1 = 2-thienyl, PhCH(NH2), PhCH2, 2-furyl; R2, R3 = H, Et, allyl, Ph; NR2R3 = morpholino) were prepd.

in 41-100% yield by treatment of II with H2NNHC(:NH)NR2R3. P-nitrophenyl Prepared by M. Hale 308-4258 Page 238

3-formyl-7-tert-butoxycarbonylamino-3-cephem-4-carboxylate reacted with 4,4-(3-oxopentamethylene)guanylhydrazine-HBr and THF for 16.5 hr at room temp. to give 72% of the

3-[[4,4-(3-oxopentamethylene)guanylhydrazono]meth yl] cephem deriv.

L3 ANSWER 132 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 56204-11-6 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
3-[(imino-4-morpholinylmethyl)hydrazono]methyl]-7-[[[(1-methyl-1H-tetrazol-5-yl)thio]acetyl]amino]-8-oxo-, monohydrobromide, (6R-trans)-(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C17 H22 N10 O5 S2 . Br H

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry unknown.

• HBr

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 83:58855 Pharmaceutical cephalosporins. Yoshioka, Mitsuru; Sendo, Yuji; Murakami, Masayuki; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). Ger. Offen. DE 2450618 19750430, 56 pp. (German).

CODEN: GWXXBX. PRIORITY: JP 1973-120328 19731025.

GI For diagram(s), see printed CA Issue.

AB Approx. 60 bactericides (no data) I (e.g., R1 = 2-thienyl, PhCH(NH2), PhCH2, 2-furyl; R2, R3 = H, Et, allyl, Ph; NR2R3 = morpholino) were prepd.

in 41-100% yield by treatment of II with H2NNHC(:NH)NR2R3. P-nitrophenyl 3-formyl-7-tert-butoxycarbonylamino-3-cephem-4-carboxylate reacted with 4,4-(3-oxopentamethylene)guanylhydrazine-HBr and THF for 16.5 hr at room temp. to give 72% of the

3-[[4,4-(3-oxopentamethylene)guanylhydrazono]meth

yl] cephem deriv.

Prepared by M. Hale 308-4258

L3 ANSWER 133 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 56204-10-5 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
3-[[(imino-4-morpholinylmethyl)hydrazono]methyl]-8-oxo-7[(phenoxyacetyl)amino]-, monohydrobromide, (6R-trans)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C21 H24 N6 O6 S . Br H

LC STN Files: CA, CAPLUS

CRN (62733-27-1)

Absolute stereochemistry.
Double bond geometry unknown.

• HBr

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 83:58855 Pharmaceutical cephalosporins. Yoshioka, Mitsuru; Sendo, Yuji; Murakami, Masayuki; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). Ger. Offen. DE 2450618 19750430, 56 pp. (German).

CODEN: GWXXBX. PRIORITY: JP 1973-120328 19731025.

GI For diagram(s), see printed CA Issue.

AB Approx. 60 bactericides (no data) I (e.g., R1 = 2-thienyl, PhCH(NH2), PhCH2, 2-furyl; R2, R3 = H, Et, allyl, Ph; NR2R3 = morpholino) were prepd.

in 41-100% yield by treatment of II with H2NNHC(:NH)NR2R3. P-nitrophenyl 3-formyl-7-tert-butoxycarbonylamino-3-cephem-4-carboxylate reacted with 4,4-(3-oxopentamethylene)guanylhydrazine-HBr and THF for 16.5 hr at room temp. to give 72% of the

3-[[4,4-(3-oxopentamethylene)guanylhydrazono]meth yl] cephem deriv.

L3 ANSWER 134 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 56204-07-0 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
3-[(imino-4-thiomorpholinylmethyl)hydrazono]methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, monohydriodide, (6R-trans)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:

Prepared by M. Hale 308-4258

CN Thiomorpholine, 5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid deriv.

FS STEREOSEARCH

MF C19 H22 N6 O4 S3 . H I

LC STN Files: CA, CAPLUS

CRN (62733-26-0)

Absolute stereochemistry.
Double bond geometry unknown.

HI

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 83:58855 Pharmaceutical cephalosporins. Yoshioka, Mitsuru; Sendo, Yuji; Murakami, Masayuki; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). Ger. Offen. DE 2450618 19750430, 56 pp. (German).

CODEN: GWXXBX. PRIORITY: JP 1973-120328 19731025.

GI For diagram(s), see printed CA Issue.

AB Approx. 60 bactericides (no data) I (e.g., R1 = 2-thienyl, PhCH(NH2), PhCH2, 2-furyl; R2, R3 = H, Et, allyl, Ph; NR2R3 = morpholino) were prepd.

in 41-100% yield by treatment of II with H2NNHC(:NH)NR2R3. P-nitrophenyl 3-formyl-7-tert-butoxycarbonylamino-3-cephem-4-carboxylate reacted with 4,4-(3-oxopentamethylene)guanylhydrazine-HBr and THF for 16.5 hr at room temp. to give 72% of the

3-[[4,4-(3-oxopentamethylene)guanylhydrazono]meth yl] cephem deriv.

L3 ANSWER 135 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 56204-06-9 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[(imino-3-thiazolidinylmethyl)hydrazono]methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, monohydriodide, (6R-trans)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C18 H20 N6 O4 S3 . H I

LC STN Files: CA, CAPLUS

CRN (62733-25-9)

Absolute stereochemistry. Prepared by M. Hale 308-4258

Double bond geometry unknown.

• H]

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 83:58855 Pharmaceutical cephalosporins. Yoshioka, Mitsuru; Sendo, Yuji; Murakami, Masayuki; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). Ger. Offen. DE 2450618 19750430, 56 pp. (German).

CODEN: GWXXBX. PRIORITY: JP 1973-120328 19731025.

GI For diagram(s), see printed CA Issue.

AB Approx. 60 bactericides (no data) I (e.g., R1 = 2-thienyl, PhCH(NH2), PhCH2, 2-furyl; R2, R3 = H, Et, allyl, Ph; NR2R3 = morpholino) were prepd.

in 41-100% yield by treatment of II with H2NNHC(:NH)NR2R3. P-nitrophenyl 3-formyl-7-tert-butoxycarbonylamino-3-cephem-4-carboxylate reacted with 4,4-(3-oxopentamethylene)guanylhydrazine-HBr and THF for 16.5 hr at room temp. to give 72% of the

3-[[4,4-(3-oxopentamethylene)guanylhydrazono]meth yl] cephem deriv.

L3 ANSWER 136 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 56204-05-8 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

3-[[[(dihydro-2H-1,3-oxazin-3(4H)-yl)iminomethyl]hydrazono]methyl]-8-oxo-7[(2-thienylacetyl)amino]-, monohydriodide, (6R-trans)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2H-1,3-Oxazine, 5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid deriv.

FS STEREOSEARCH

MF C19 H22 N6 O5 S2 . H I

LC STN Files: CA, CAPLUS

CRN (62733-24-8)

нт

- 1 REFERENCES IN FILE CA (1967 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 83:58855 Pharmaceutical cephalosporins. Yoshioka, Mitsuru; Sendo, Yuji; Murakami, Masayuki; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). Ger. Offen. DE 2450618 19750430, 56 pp. (German).

CODEN: GWXXBX. PRIORITY: JP 1973-120328 19731025.

GI For diagram(s), see printed CA Issue.

AB Approx. 60 bactericides (no data) I (e.g., R1 = 2-thienyl, PhCH(NH2), PhCH2, 2-furyl; R2, R3 = H, Et, allyl, Ph; NR2R3 = morpholino) were prepd.

in 41-100% yield by treatment of II with H2NNHC(:NH)NR2R3. P-nitrophenyl 3-formyl-7-tert-butoxycarbonylamino-3-cephem-4-carboxylate reacted with 4,4-(3-oxopentamethylene)guanylhydrazine-HBr and THF for 16.5 hr at room temp. to give 72% of the

3-[[4,4-(3-oxopentamethylene)guanylhydrazono]meth yl] cephem deriv.

- L3 ANSWER 137 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 56204-04-7 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

3-[[[imino(tetrahydro-2H-1,2-oxazin-2-yl)methyl]hydrazono]methyl]-8-oxo-7 [(2-thienylacetyl)amino]-, monohydriodide, (6R-trans)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2H-1,2-Oxazine, 5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid deriv.

FS STEREOSEARCH

MF C19 H22 N6 O5 S2 . H I

LC STN Files: CA, CAPLUS

CRN (62733-23-7)

• н.

- 1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)
- REFERENCE 1: 83:58855 Pharmaceutical cephalosporins. Yoshioka, Mitsuru; Sendo, Yuji; Murakami, Masayuki; Miyazaki, Sadao; Ishikura, Koji (Shionogi
- and Co., Ltd., Japan). Ger. Offen. DE 2450618 19750430, 56 pp. (German).
 - CODEN: GWXXBX. PRIORITY: JP 1973-120328 19731025.
- GI For diagram(s), see printed CA Issue.
- AB Approx. 60 bactericides (no data) I (e.g., R1 = 2-thienyl, PhCH(NH2), PhCH2, 2-furyl; R2, R3 = H, Et, allyl, Ph; NR2R3 = morpholino) were prepd.
 - in 41-100% yield by treatment of II with H2NNHC(:NH)NR2R3. P-nitrophenyl 3-formyl-7-tert-butoxycarbonylamino-3-cephem-4-carboxylate reacted with 4,4-(3-oxopentamethylene)guanylhydrazine-HBr and THF for 16.5 hr at room temp. to give 72% of the
- 3-[[4,4-(3-oxopentamethylene)guanylhydrazono]meth yl] cephem deriv.
- L3 ANSWER 138 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 56204-03-6 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
- 3-[[(2,6-dimethyl-4-morpholinyl)iminomethyl]hydrazono]methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, monohydriodide, [6R-(6.alpha.,7.beta.)]- (9CI) (CA
 - INDEX NAME)
- FS STEREOSEARCH
- MF C21 H26 N6 O5 S2 . H I
- LC STN Files: CA, CAPLUS
- CRN (62777-35-9)

• HI

- 1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)
- REFERENCE 1: 83:58855 Pharmaceutical cephalosporins. Yoshioka, Mitsuru; Sendo, Yuji; Murakami, Masayuki; Miyazaki, Sadao; Ishikura, Koji (Shionogi
- and Co., Ltd., Japan). Ger. Offen. DE 2450618 19750430, 56 pp. (German).
 - CODEN: GWXXBX. PRIORITY: JP 1973-120328 19731025.
- GI For diagram(s), see printed CA Issue.
- AB Approx. 60 bactericides (no data) I (e.g., R1 = 2-thienyl, PhCH(NH2), PhCH2, 2-furyl; R2, R3 = H, Et, allyl, Ph; NR2R3 = morpholino) were prepd.
 - in 41-100% yield by treatment of II with H2NNHC(:NH)NR2R3. P-nitrophenyl 3-formyl-7-tert-butoxycarbonylamino-3-cephem-4-carboxylate reacted with 4,4-(3-oxopentamethylene)guanylhydrazine-HBr and THF for 16.5 hr at room temp. to give 72% of the
- 3-[[4,4-(3-oxopentamethylene)guanylhydrazono]meth yl] cephem deriv.
- L3 ANSWER 139 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 56204-02-5 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
- 3-[[((2,5-dimethyl-4-morpholinyl)iminomethyl]hydrazono]methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, monohydriodide, [6R-(6.alpha.,7.beta.)]- (9CI)
 (CA

INDEX NAME)

- FS STEREOSEARCH
- MF C21 H26 N6 O5 S2 . H I
- LC STN Files: CA, CAPLUS
- CRN (62777-34-8)

• HI

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 83:58855 Pharmaceutical cephalosporins. Yoshioka, Mitsuru; Sendo, Yuji; Murakami, Masayuki; Miyazaki, Sadao; Ishikura, Koji (Shionoqi

and Co., Ltd., Japan). Ger. Offen. DE 2450618 19750430, 56 pp. (German).

CODEN: GWXXBX. PRIORITY: JP 1973-120328 19731025.

GI For diagram(s), see printed CA Issue.

AB Approx. 60 bactericides (no data) I (e.g., R1 = 2-thienyl, PhCH(NH2), PhCH2, 2-furyl; R2, R3 = H, Et, allyl, Ph; NR2R3 = morpholino) were prepd.

in 41-100% yield by treatment of II with H2NNHC(:NH)NR2R3. P-nitrophenyl 3-formyl-7-tert-butoxycarbonylamino-3-cephem-4-carboxylate reacted with 4,4-(3-oxopentamethylene)guanylhydrazine-HBr and THF for 16.5 hr at room temp. to give 72% of the

3-[[4,4-(3-oxopentamethylene)guanylhydrazono]meth yl] cephem deriv.

L3 ANSWER 140 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 56204-01-4 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[[[imino(3-methyl-4-morpholinyl)methyl]hydrazono]methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, monohydriodide, [6R-(6.alpha.,7.beta.)]- (9CI)

(CA INDEX NAME)

FS STEREOSEARCH

MF C20 H24 N6 O5 S2 . H I

LC STN Files: CA, CAPLUS

CRN (62777-33-7)

H1

- 1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)
- REFERENCE 1: 83:58855 Pharmaceutical cephalosporins. Yoshioka, Mitsuru; Sendo, Yuji; Murakami, Masayuki; Miyazaki, Sadao; Ishikura, Koji (Shionogi
- and Co., Ltd., Japan). Ger. Offen. DE 2450618 19750430, 56 pp. (German).
 - CODEN: GWXXBX. PRIORITY: JP 1973-120328 19731025.
- GI For diagram(s), see printed CA Issue.
- AB Approx. 60 bactericides (no data) I (e.g., R1 = 2-thienyl, PhCH(NH2), PhCH2, 2-furyl; R2, R3 = H, Et, allyl, Ph; NR2R3 = morpholino) were prepd.
 - in 41-100% yield by treatment of II with H2NNHC(:NH)NR2R3. P-nitrophenyl 3-formyl-7-tert-butoxycarbonylamino-3-cephem-4-carboxylate reacted with 4,4-(3-oxopentamethylene)guanylhydrazine-HBr and THF for 16.5 hr at room temp. to give 72% of the
- 3-[[4,4-(3-oxopentamethylene)guanylhydrazono]meth yl] cephem deriv.
- L3 ANSWER 141 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 56204-00-3 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
 3-[[imino(2-methyl-4-morpholinyl)methyl]hydrazono]methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, [6R-(6.alpha.,7.beta.)]- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C20 H24 N6 O5 S2
- CI COM
- LC STN Files: BEILSTEIN*, CA, CAPLUS
 (*File contains numerically searchable property data)

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 83:58855 Pharmaceutical cephalosporins. Yoshioka, Mitsuru; Sendo, Yuji; Murakami, Masayuki; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). Ger. Offen. DE 2450618 19750430, 56 pp. (German).

CODEN: GWXXBX. PRIORITY: JP 1973-120328 19731025.

GI For diagram(s), see printed CA Issue.

AB Approx. 60 bactericides (no data) I (e.g., R1 = 2-thienyl, PhCH(NH2), PhCH2, 2-furyl; R2, R3 = H, Et, allyl, Ph; NR2R3 = morpholino) were prepd.

in 41-100% yield by treatment of II with H2NNHC(:NH)NR2R3. P-nitrophenyl 3-formyl-7-tert-butoxycarbonylamino-3-cephem-4-carboxylate reacted with 4,4-(3-oxopentamethylene)guanylhydrazine-HBr and THF for 16.5 hr at room temp. to give 72% of the

3-[[4,4-(3-oxopentamethylene)guanylhydrazono]meth yl] cephem deriv.

L3 ANSWER 142 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 56203-99-7 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[[[(ethylamino)-4-morpholinylmethylene]hydrazono]methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, monohydriodide, (6R-trans)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C21 H26 N6 O5 S2 . H I

LC STN Files: CA, CAPLUS

• н.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 83:58855 Pharmaceutical cephalosporins. Yoshioka, Mitsuru; Sendo, Yuji; Murakami, Masayuki; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). Ger. Offen. DE 2450618 19750430, 56 pp. (German).

CODEN: GWXXBX. PRIORITY: JP 1973-120328 19731025.

GI For diagram(s), see printed CA Issue.

AB Approx. 60 bactericides (no data) I (e.g., R1 = 2-thienyl, PhCH(NH2), PhCH2, 2-furyl; R2, R3 = H, Et, allyl, Ph; NR2R3 = morpholino) were prepd.

in 41-100% yield by treatment of II with H2NNHC(:NH)NR2R3. P-nitrophenyl 3-formyl-7-tert-butoxycarbonylamino-3-cephem-4-carboxylate reacted with 4,4-(3-oxopentamethylene)guanylhydrazine-HBr and THF for 16.5 hr at room temp. to give 72% of the

3-[[4,4-(3-oxopentamethylene)guanylhydrazono]meth
 yl] cephem deriv.

L3 ANSWER 143 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 56203-98-6 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[[(imino-4-morpholinylmethyl)hydrazono]methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, monohydriodide, (6R-trans)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C19 H22 N6 O5 S2 . H I

LC STN Files: CA, CAPLUS

CRN (62733-20-4)

H.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 83:58855 Pharmaceutical cephalosporins. Yoshioka, Mitsuru; Sendo, Yuji; Murakami, Masayuki; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). Ger. Offen. DE 2450618 19750430, 56 pp. (German).

CODEN: GWXXBX. PRIORITY: JP 1973-120328 19731025.

GI For diagram(s), see printed CA Issue.

AB Approx. 60 bactericides (no data) I (e.g., R1 = 2-thienyl, PhCH(NH2), PhCH2, 2-furyl; R2, R3 = H, Et, allyl, Ph; NR2R3 = morpholino) were prepd.

in 41-100% yield by treatment of II with H2NNHC(:NH)NR2R3. P-nitrophenyl 3-formyl-7-tert-butoxycarbonylamino-3-cephem-4-carboxylate reacted with 4,4-(3-oxopentamethylene)guanylhydrazine-HBr and THF for 16.5 hr at room temp. to give 72% of the

3-[[4,4-(3-oxopentamethylene)guanylhydrazono]meth yl] cephem deriv.

L3 ANSWER 144 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 56203-97-5 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[[(imino-4-morpholinylmethyl)hydrazono]methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, monohydrobromide, (6R-trans)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C19 H22 N6 O5 S2 . Br H

LC STN Files: CA, CAPLUS

CRN (62733-20-4)

HBr

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 83:58855 Pharmaceutical cephalosporins. Yoshioka, Mitsuru; Sendo, Yuji; Murakami, Masayuki; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). Ger. Offen. DE 2450618 19750430, 56 pp. (German).

CODEN: GWXXBX. PRIORITY: JP 1973-120328 19731025.

GI For diagram(s), see printed CA Issue.

AB Approx. 60 bactericides (no data) I (e.g., R1 = 2-thienyl, PhCH(NH2), PhCH2, 2-furyl; R2, R3 = H, Et, allyl, Ph; NR2R3 = morpholino) were prepd.

in 41-100% yield by treatment of II with H2NNHC(:NH)NR2R3. P-nitrophenyl 3-formyl-7-tert-butoxycarbonylamino-3-cephem-4-carboxylate reacted with 4,4-(3-oxopentamethylene)guanylhydrazine-HBr and THF for 16.5 hr at room temp. to give 72% of the

3-[[4,4-(3-oxopentamethylene)guanylhydrazono]meth yl] cephem deriv.

- L3 ANSWER 145 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 56203-96-4 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[[(hexahydro-1H-azepin-1-yl)iminomethyl]hydrazono]methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, monohydriodide, (6R-trans)- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C21 H26 N6 O4 S2 . H I
- LC STN Files: CA, CAPLUS

• HI

- 1 REFERENCES IN FILE CA (1967 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 83:58855 Pharmaceutical cephalosporins. Yoshioka, Mitsuru; Sendo, Yuji; Murakami, Masayuki; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). Ger. Offen. DE 2450618 19750430, 56 pp. (German).

CODEN: GWXXBX. PRIORITY: JP 1973-120328 19731025.

GI For diagram(s), see printed CA Issue.

AB Approx. 60 bactericides (no data) I (e.g., R1 = 2-thienyl, PhCH(NH2), PhCH2, 2-furyl; R2, R3 = H, Et, allyl, Ph; NR2R3 = morpholino) were prepd.

in 41-100% yield by treatment of II with H2NNHC(:NH)NR2R3. P-nitrophenyl 3-formyl-7-tert-butoxycarbonylamino-3-cephem-4-carboxylate reacted with 4,4-(3-oxopentamethylene)guanylhydrazine-HBr and THF for 16.5 hr at room temp. to give 72% of the

3-[[4,4-(3-oxopentamethylene)guanylhydrazono]meth yl] cephem deriv.

- L3 ANSWER 146 OF 148 REGISTRY COPYRIGHT 2000 ACS
- RN 56203-95-3 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[[(3,6-dihydro-1(2H)-pyridinyl)iminomethyl]hydrazono]methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, (6R-trans)- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C20 H22 N6 O4 S2

LC STN Files: BEILSTEIN*, CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL (*File contains numerically searchable property data)

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 86:189975 Cephalosporin compounds. Yoshioka, Mitsuru; Murakami, Masayuki; Sendo, Yuji; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). U.S. US 3997528 19761214, 23 pp. (English). CODEN: USXXAM. PRIORITY: JP 1973-12032 19731025.

GΙ

AB The antibacterial (no data) (guanylhydrazono)cephalosporins I (R, R1, R2

alkyl, alkenyl, aralkyl, aryl, NH2, MeO; NR1R2 = N-heterocyclic, i.e. morpholino, piperidino; RR1 = CH2CH2; R3 = H, thienylacetyl, PhOCH2CO, H2NCHPhCO, PhCH2CO, furylacetyl, tetrazolylacetyl, Me3CCO2C, Cl3CCH2O2C; R4 = H; n = 1, 0) and their salts were prepd. by treating the hemiacetal lactones II with H2NNHC(NR1R2):NR (III). I (R4 = 4-O2NC6H4CH2, Ph2CH,

Me)

were prepd. by treating 3-formylcephem-4-carboxylates with III.

REFERENCE 2: 83:58855 Pharmaceutical cephalosporins. Yoshioka, Mitsuru; Sendo, Yuji; Murakami, Masayuki; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). Ger. Offen. DE 2450618 19750430, 56 pp. (German).

CODEN: GWXXBX. PRIORITY: JP 1973-120328 19731025.

GI For diagram(s), see printed CA Issue.

AB Approx. 60 bactericides (no data) I (e.g., R1 = 2-thienyl, PhCH(NH2), PhCH2, 2-furyl; R2, R3 = H, Et, allyl, Ph; NR2R3 = morpholino) were prepd.

in 41-100% yield by treatment of II with H2NNHC(:NH)NR2R3. P-nitrophenyl 3-formyl-7-tert-butoxycarbonylamino-3-cephem-4-carboxylate reacted with Prepared by M. Hale 308-4258 Page 253

4,4-(3-oxopentamethylene)guanylhydrazine-HBr and THF for 16.5 hr at room temp. to give 72% of the

3-[[4,4-(3-oxopentamethylene)guanylhydrazono]meth yl] cephem deriv.

L3 ANSWER 147 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 56203-94-2 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,

3-[[[(2,5-dihydro-1H-pyrrol-1-yl)iminomethyl]hydrazono]methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, monohydriodide, (6R-trans)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C19 H20 N6 O4 S2 . H I

LC STN Files: CA, CAPLUS

CRN (62733-18-0)

Absolute stereochemistry. Double bond geometry unknown.

● HI

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 83:58855 Pharmaceutical cephalosporins. Yoshioka, Mitsuru; Sendo, Yuji; Murakami, Masayuki; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). Ger. Offen. DE 2450618 19750430, 56 pp. (German).

CODEN: GWXXBX. PRIORITY: JP 1973-120328 19731025.

GI For diagram(s), see printed CA Issue.

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3-[[4,4-(3-oxopentamethylene)guanylhydrazono]meth yl] cephem deriv.

L3 ANSWER 148 OF 148 REGISTRY COPYRIGHT 2000 ACS

RN 56203-93-1 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, Prepared by M. Hale 308-4258

3-[[(imino-1-pyrrolidinylmethyl)hydrazono]methyl]-8-oxo-7-[(2-thienylacetyl)amino]-, monohydrobromide, (6R-trans)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C19 H22 N6 O4 S2 . Br H

LC STN Files: CA, CAPLUS

CRN (62733-16-8)

Absolute stereochemistry.
Double bond geometry unknown.

• HBr

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 83:58855 Pharmaceutical cephalosporins. Yoshioka, Mitsuru; Sendo, Yuji; Murakami, Masayuki; Miyazaki, Sadao; Ishikura, Koji (Shionogi

and Co., Ltd., Japan). Ger. Offen. DE 2450618 19750430, 56 pp. (German).

CODEN: GWXXBX. PRIORITY: JP 1973-120328 19731025.

GI For diagram(s), see printed CA Issue.

AB Approx. 60 bactericides (no data) I (e.g., R1 = 2-thienyl, PhCH(NH2), PhCH2, 2-furyl; R2, R3 = H, Et, allyl, Ph; NR2R3 = morpholino) were prepd.

in 41-100% yield by treatment of II with H2NNHC(:NH)NR2R3. P-nitrophenyl 3-formyl-7-tert-butoxycarbonylamino-3-cephem-4-carboxylate reacted with 4,4-(3-oxopentamethylene)guanylhydrazine-HBr and THF for 16.5 hr at room temp. to give 72% of the

3-[[4,4-(3-oxopentamethylene)guanylhydrazono]meth yl] cephem deriv.

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Prepared by M. Hale 308-4258

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